2023 IEEE 13th International Conference "Nanomaterials: Applications & Properties" (IEEE NAP – 2023)
Bratislava, Slovakia September 10-15, 2023

Institute of Electrical Engineering
Slovak Academy of Sciences
Slovak University of Technology in Bratislava
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IEEE Nanotechnology Council

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NANOmaterials: Applications & Properties -2023

ABSTRACTS BOOK

Institute of Electrical and Electronics Engineers
2023

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Book of Abstracts

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TRACK 1

“NANOMATERIALS SYNTHESIS & SELF-ASSEMBLY”

Facile One-Step Hydrothermal Synthesis of Monolayer and Turbostratic Bilayer *n*-doped Graphene Quantum Dots Using Sucrose as a Carbon Source

Akkawat Ruammaitree*
Department of Physics, Faculty of Science and Technology, Thammasat University (Thailand)
* u4605070@hotmail.com

Abstract ID #NSS-0466

Graphene quantum dots (GQDs) have attracted attention from researchers due to their outstanding properties, such as chemical inertness, stable photoluminescence (PL), biocompatibility, low toxic, which make them suitable for bioimaging, optoelectronic device, sensor and so on. At present, there are many publications report the effect of size of GQDs on their properites but there is hardly any publication reports the effect of thickness of GQDs on their properties. It may be attributed to the difficulty to obtain the accurate information on the thickness of GQDs. In this report, we demonstrate the facile and one-step hydrothermal synthesis of monolayer and bilayer n-doped graphene quantum dots (NGQDs) using sucrose as a carbon source. UV-visible and PL spectra show the quantum yield of the NGQDs is 4.9 times higher than that of the GQDs. Besides, the NGQDs exhibit sensitive PL for Ag^+ ions. In addition, the thickness distribution and interlayer spacing of NGQDs are revealed by X-ray diffraction (XRD) curve ftting which is calculated using a simple and accurate equation. The information on the structure of the NGQDs from the XRD curve ftting is in a good agreement with the Raman results.

ACKNOWLEDGMENTS

This work was supported by the Thailand Science Research and Innovation Fundamental Fund fiscal year 2023, and Thammasat University Research Fund, Contract No. TUFT 7/2564, and Thammasat University Research Unit in Synthesis and Applications of Graphene.

Structure Property Relationships for Thermostable Nanocomposites Based on Poly(benzoxazine-co-cyanate ester resin) and Functionalized Polyhedral Oligomeric Silsesquioxanes

Diana Shulzhenko[1 *], Olga Starostenko[1], Olga Grigoryeva[1], Alexander Fainleib[1], Daniel Grande[2]
[1] *Institute of Macromolecular Chemistry, NAS of Ukraine (Ukraine)*
[2] *Institut de Chimie et des Matériaux Paris-Est (France)*
* darkblue1cherry2black@gmail.com

Abstract ID #NSS -0476

In recent decades, heat-resistant polymer nanocomposites synthesized in situ based on thermosetting monomers and 3D nanosized polyhedral oligomeric silsesquioxanes (POSS) containing surface functional groups that are reactive with respect to the monomer and to the emerging polymer have attracted great interest. The present research is focused on the synthesis and thermal properties of novel high-performance thermostable nanocomposites based on copolymer of cyanate ester resin (CER) with benzoxazine (BOA) and the functionalized POSS.

The nanosized functionalized POSS, viz. aminoethylaminopropylisobutyl POSS (AEAPIB-POSS) and epoxycyclohexyl-POSS (ECH-POSS) were used as nanofillers with content of 0.05 wt.%. The chemical grafting of POSS nanoparticles to the poly(CER-co-BOA) network via reaction of amino- or epoxy-groups is evidenced by FTIR spectroscopy measurements.

The filled compositions were cured from 20 to 300 ºC at a heating rate of 0.5 ºC/min and final nanocomposites were assigned as poly(CER-co-BOA)/AEAPIB-POSS and poly(CER-co-BOA)/ECH-POSS. For comparison, a sample of unfilled poly(CER-co-BOA) was synthesized in the same curing schedule. The ratio between CER and BOA was equal to 75:25 wt.% for all the compositions synthesized.

Differential scanning calorimetry (DSC) with DSC 25 apparatus (TA Instruments, USA) was used for estimating glass transition temperatures, Tg, in the composites over the temperature range from 25°C to 350 °C. The thermal stability of composites after complete polymerization was determined using a SETSYS Evolution TGA 16 thermobalance (SETARAM, France), with a platinum pan under 20 mL/min argon flow rate at a heating rate of 20 °C/min from 50 °C to 800 °C.

DSC measurements have shown that in comparison to the unfilled poly(CER-co-BOA) the Tg value of the poly(CER-co-BOA)/AEAPIB-POSS and poly(CER-co-BOA)/ECH-POSS nanocomposites shifted to higher temperature from 193 °C to 204 °C and 207°C, respectively. TGA investigation has shown that even at such extra low content of the nanofiller the poly(CER-co-BOA)/AEAPIB-POSS and poly(CER-co-BOA)/ECH-POSS nanocomposites exhibit higher thermal stability compared to p(CER-co-BOA) sample.

It can be concluded that the use of ultra-low additions of both functionalized POSS (ECH-POSS and AEAPIB-POSS) is effective in enhancing the thermal performance of poly(CER-co-BOA)/POSS nanocomposites.

ACKNOWLEDGMENTS

The authors are indebted to the National Academy of Sciences of Ukraine and Centre National de la Recherche Scientifique of France for financial support through POLYTHERMAT International Research Project.

Synthesis of Superhydrophobic Coating Reinforced with Nano Materials Dispersed in Polymer Matrix for Flexible Electronics Applications

Dr Meena Sadashiv Laad[1*], Akhila Vaman Shalu1[1]
Symbiosis International University (India)
* meena@sitpune.edu.in

Abstract ID #NSS -0484

Demand for superhydrophobic coatings is rising in textiles, wearable electronics, and healthcare implants owing to their non-wetting, bacterial-resistant, icing-resistance, and self-cleaning qualities. Considering the promising applications of superhydrophobic materials in consumer electronics, there is a significant need to create novel materials and fabrication methods that can be used to fabricate high-performance scalable electronic devices that can be directly mounted on conductive and flexible substrates for a variety of applications. The discovery of conducting polymers, amorphous silicon, and organic semiconductors has provided the base material for fabricating flexible electronic devices which are bendable, rollable, stretchable, and foldable, some of the important properties which the conventional rigid electronic materials failed to offer. Super-hydrophobic materials with superior electrical conductivity and high stretchability have a variety of uses in wearable electronics, including as sensors, energy storage systems, anti-corrosion circuits, etc.

In the present work, a superhydrophobic conductive film is fabricated by depositing a polymer matrix solution containing (Multi walled carbon nanotubes) MWCNTs and SEBS copolymer along with Fe_3O_4 and nano-silica as secondary fillers on an OHP sheet. A water contact angle of 154° was attained with an electrical resistance of 500Ω, confirming the optimum value of the degree of superhydrophobicity and conductivity of the fabricated film.

ACKNOWLEDGMENTS

The authors acknowledge Symbiosis International University, Pune, India for providing research funding to carry out the present research work.

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Pulsed Laser Ablation Synthesis of $CeAlO_3$ Nanocrystals

Volodymyr Vasylkovskyi[1*], Iryna Bespalova[1], Mykola Slipchenko[1], Olena Slipchenko[2], Oleksandr Sorokin[1], Oleg Sidletskiy[1], Iaroslav Gerasymov[1], Pavlo Arhipov[1], Serhii Tkachenko[1]
[1] "*Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry (Romania)*
[2] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[3] *National Technical University – «Kharkiv Polytechnic Institute» (Ukraine)*
* vasylkovskyi.volodymyr@gmail.com

Abstract ID #NSS-0490

Pulsed laser ablation (PLA) technique is a "green" physical alternative to conventional chemical methods and gaining attention for its ability to produce nanomaterials, with a highly pure surface, in a vacuum, gas, or liquid media. The size and shape of the obtained nanomaterials can be controlled by adjusting the laser parameters and environment of the PLA process. PLA has been used to fabricate a variety of nanomaterials including metals, semiconductors, ceramics, alloys, and scintillation materials. A scintillator is a type of material that converts various kinds of high-energy radiation into near-visible or visible light. Such materials are usually applied as single crystals and used as detectors in high-energy physics, medical diagnostics, security applications, etc. But scintillators in the form of nanomaterials are not widely used. Also, the PLA technique was not applied to the fabrication of scintillation nanocrystals (NCs) with perovskite structure until now. The study shows that using the PLA technique the CeAlO3 [1,2] NCs with a perovskite crystalline lattice with improved optical properties can be fabricated. The geometrical (transmission electron microscopy), composition (X-ray diffraction analysis, X-Ray photoelectron spectroscopy), and optical (luminescence, luminescent decay times measurements) parameters of obtained CeAlO3 NCs were investigated. The retaining of crystalline structure and materials composition as well as the improvement of optical properties compared to the bulk material are demonstrated. The obtained NCs with an average size of 5.5 nm showed the shortening of luminescence decay times. The research opens new possibilities for the physical synthesis of perovskite nanocrystals for the fabrication of new scintillation structures with improved properties.

ACKNOWLEDGMENTS

This work was supported by the Federal Ministry of Education and Research of Germany in the framework of the project "German-Ukrainian Cores of Excellence" - «NanoScint» (01DK21007) and German Academic Exchange Service – "Research Grants - Short-Term Grants" (57552337). Thanks go to the Laboratory of Nano and Quantum Engineering (LNQE) of Leibniz University Hannover for the possibility of conducting TEM measurements.

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Synthesis of Functional Nanocomposites and Nanohybrids Based on the Nanoscale Oxide Materials

Anatolii Belous*, Ivan Lisovskyi, Pavlo Torchyniuk, Yuliia Shlapa
V. Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine (Ukraine)
* agbilous@ukr.net

Abstract ID #NSS-0497

Nanocomposites and nanohybrids have been attracting significant scientific and practical interest due to the possibility of combining various useful properties in one material and increasing its functionality. Such systems can find practical application both in technology (magnetic recording systems, elements of microwave technology, electrochemical systems) and in medicine (MRI, hyperthermia, drugs delivery). The synthesis of non-agglomerated or weakly agglomerated nanoparticles and the development of special-purpose nanocomposites based on them is a serious scientific task. The preparation of such composites depends essentially on the chemical composition of nanoparticles, their crystalline structure and physical-chemical properties, as well as on the method of synthesis.

The aim of this work was the synthesis of weakly agglomerated nanoparticles of various materials, in particular, ferrites based on complex oxide systems with spinel, perovskite, and barium hexaferrite structures; lithium-conducting systems with NASICON, perovskite and garnet structures, and also organic-inorganic perovskites. Such methods as precipitation in aqueous and non-aqueous solutions, inverse microemulsion, sol-gel, and spin-coating were used for the synthesis of materials. The relationships between the chemical composition, crystalline structure, and conditions of synthesis of weakly agglomerated nanoparticles were established. Synthesized nanoparticles were used to prepare functional nanohybrid materials for various purposes (hybrid magnetic films for microwave resonators, lithium-conductive films for lithium-ion batteries, organic-inorganic perovskites films for solar cells), and also nanocomposites with core/shell structure. Optimal methods for manufacturing structured nanocomposite and nanohybrid materials with controlled physical-chemical parameters were established. It has been shown that the synthesized composite materials possess an increased functional effect compared to existing nanoparticles. These composite materials can be used for the fabrication of controlled microwave resonant elements, for the development of electrochemical and photovoltaic systems, and also for medical and biological purposes.

ACKNOWLEDGMENTS

This work was partially supported by grant G6002 within the NATO Science for Peace and Security Programme.

Fabrication of Nanocomposites Based on the Activated Carbon and CeO_2 Nanoparticles for Biomedical Application

Yuliia Shlapa[1*], Veronika Sarnatskaya[2], Serhii Solopan[1], Bogdan Gerashchenko[2], Oleksii Sydorenko[2], Dmytro Klymchuk[3], Anatolii Belous[1]

[1] *V.Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine (Ukraine)*
[2] *R. E. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology of the NAS of Ukraine (Ukraine)*
[3] *M.G. Kholodny Institute of Botany of the NAS of Ukraine (Ukraine)*

* yuliashlapa@ukr.net

Abstract ID #NSS -0498

CeO_2 nanoparticles (NPs) are being of great scientific interest in biomedicine due to their unique ability to scavenge the reactive oxygen species (ROS) and mitigate different manifistations of the oxidative stress, which accompains various diseases including the acute radiation sickness. The challenging scientific issue is to enhance the activity of CeO_2 NPs by their binding with other types of functional materials. One of the such possible materials is the carbon particles with ultra-high adsorption properties, which are able to adsorb endo- and exogenous metabolites and toxins accumulated together with the ROS and the end products of protein and lipid oxidation. Fabrication of such carbon/CeO2 composite can provide the possibility to combine the sorption potential and antioxidant properties in the same material and make it promising for application in biomedical studies. The aim of this work was to fabricate the "C@CeO_2" composite, to study its morphology and physical-chemical properties, and examine its bioeffects.

Two methods of synthesis of C@CeO_2 composites, namely i) mechanical mixing of the individual components (C@CeO_2-1) using the planetary mill and ii) hydrothermal synthesis (C@CeO_2-2), were used within this work. Noteworthy that carbon particles used for the hydrothermal synthesis of composite were preliminary grinded in the planetary mill at chosen suitable conditions followed by the oxidation with H_2O_2. XRD, FTIR, TEM and DLS data confirmed the co-existance of both carbon and CeO2 in the fabricated composites. Obtained results reveal that the method of synthesis significantly affects the morphology and physical-chemical properties of C@CeO2 composites. TEM data have demonstrated that in C@CeO_2-1 sample CeO_2 NPs with an average size of 15 nm are distributed on the surface of the amorphous carbon particles, while C@CeO_2-2 composite looks like the homogeneous mechanical mixture consisting of mostly crystalline NPs with the multiple morphology. Both C@CeO_2-1 and C@CeO_2-2 samples form highly-stable aqueous suspensions in opposite to the initial carbon particles. Their zeta-potential values significantly depend on the method of synthesis and equal +32.9 mV and -32.1 mV, respectively. It should be mentioned that oxidized carbon particles also formed the highly-stable suspension (ζ=-42.5 mV) mainly due to the presence of surface oxygen groups. Complex physical-chemical data proposed the formation of the composites via different mechanism dependently on the chosen method of synthesis.

Both C@CeO_2-1 and C@CeO_2-2 composites at concentrations of 3 – 200 μg/ml (determined on the basis of light absorbance of carbon) did not cause any toxic effects and did not affect proliferation of the mouse bone marrow cells (MBMC) or mouse aortic endothelial cells (MAEC). The number of live cells in both cell lines did not differ from that in the intact control of corresponding cell lines after their incubation with testing suspensions of nanocomposites.

ACKNOWLEDGMENTS

This work was performed within the NATO Science for Peace and Security Programme (grant G5683).

Effect of Multi-Walled Carbon Nanotubes on the Microhardness of Iron-Copper Nanocomposites

Mykola Melnichenko[1 *], Sergiy Revo[1], Yaroslav Zhuk[1]
Taras Shevchenko National University of Kyiv (Ukraine)
* realcrystallab@univ.kiev.ua

Abstract ID #NSS-0502

The use of mechanochemical activation of metal powders and their mixtures in planetary mills opens wide prospects for the creation of new nanocomposite materials. Mechanochemical synthesis provides the possibility of obtaining a uniform distribution of the dispersed phase, of expanding the solubility limits of elements, of reducing the grain size to the nanoscale, and of obtaining new crystalline and quasi-crystalline phases. In addition, mechanical grinding makes it is possible to obtain amorphous materials and ensure the flow of chemical reactions at low temperatures.

Nanocomposites of iron and copper (Fe-Cu) are among the most studied metastable systems obtained by mechanochemical activation of powders in a planetary mill. At the same time, nanocomposites of iron and copper are ideal model alloys for establishing patterns of structure formation and physicochemical characteristics of nanocomposite materials. However, it should be noted that the analysis of modern scientific works indicates the existence of problems in the formation of functional properties of nanocomposites based on transition metals, in particular, iron and copper with carbon nanotubes.

The paper investigated the dependence of the microhardness of Fe-Cu nanocomposites on the processing time in a planetary ball mill (20 min, 60 min, 120 min) and the influence of multi-walled carbon nanotubes on the microhardness of Fe-Cu nanocomposites with multi-walled carbon nanotubes. The research was carried out on samples of Fe-Cu nanocomposites with Fe:Cu ratio = 4:1 and 6:1 obtained in the work, undoped and doped with multi-walled carbon nanotubes (MCNT concentration was 0.5 and 1.0 vol. %). To determine the microhardness of the studied samples, a multifunctional micro-nanoindentometer "Micron-gamma" was used. The tests were carried out with loads of 100, 50, and 20 grams according to the scheme: "loading-unloading" of the indenter (without exposure). It was established that with an extension of the grinding time, the microhardness grows due to the increase in the homogeneity of the Fe-Cu nanocomposites. Results obtained in the work indicate that the presence of a small amount of multi-walled carbon nanotubes in Fe–Cu compositions obtained by mechanochemical activation in a planetary mill leads to a change in the microhardness of these materials.

It should be noted that the determination of the influence of multi-walled carbon nanotubes on microhardness is highly important from both a scientific and a practical point of view and opens up prospects for the creation of composite materials with fundamentally new physical and mechanical characteristics necessary for the use of these nanocomposites as structural materials in instrument building and the aerospace industry.

Nickel Nano-Particle Synthesis by RF Thermal Plasma Process

Chulwoong Han[1*], Sung Cheol Park[2]
[1] *Inha university & KITECH (Republic of Korea)*
[2] *KITECH (Republic of Korea)*

*hcholw@kitech.re.kr
Abstract ID #NSS-0503

Conductive metallic nano-particles are extensively used for electrical/thermal management of electronic components in the printable electronic industries[1]. Nickel nano-particle is a representative conductive metal for base metal multi-layered ceramic capacitor fabrication[2]. Ni nano-particle size has been reduced in accordance with the miniaturization trend. In this study, Ni metallic nano-particle was synthesized by feeding nickel hydroxide micro-powder into argon-hydrogen thermal plasma at different mass feeding rate. Phase, morphology, and size were investigated for as-synthesized particles. Through the results, it could be proven that nickel hydroxide feedstock particle underwent a vaporization, reduction, and condensation pathway. In addition, mean particle size was increased with feedstock mass feeding rate increasing. Higher mass feed-rate increased vapor pressure of Ni when most of feedstock powder was vaporized within the scope of this study. Accordingly, increased Ni vapor pressure raised critical condensation temperature and collision and coalescence probability between particles at relatively high temperature.

ACKNOWLEDGMENTS

"This work was supported by the Technology Innovation Program (or Industrial Stategic Technology Development Program-20019032, Development of manufacturing technology for lithium-based cathode materials with a purity of over 99% using an eco-friendly new method from secondary battery scrap black powder) funded By the Ministry of Trade, Industry & Energy(MOTIE, Korea)"

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Understanding the Properties of Nanoparticles Prepared using Solution Combustion Synthesis in a Closed Environment

Anchu Ashok[1*], Luc Vechot[2], Mamoun Al-Rawashdeh[2]
[1] *Chemical Engineering Department, Texas A&M University, Qatar (Qatar)*
[2] *Texas A&M University, Qatar (Qatar)*
* anchu.ashok@qatar.tamu.edu

Abstract ID #NSS-0507

Solution combustion technique (SCS) is a promising technique for the preparation of nanoparticles in the range of 1 -100 nm. SCS is a self-sustained reaction between the metal precursor (oxidizer) and an oxygen-containing fuel (reducer) such as urea, glycine, hydrazine, etc. in a homogeneous solution. The exothermic reaction between the fuel and the oxygen formed from the decomposition of the nitrate provides an environment for high-temperature rapid reactions that end up with the production of nanoparticles. This technique is a simple, low-cost, and energy-efficient technique for the synthesis of high-surface nanoparticles with desired properties suitable for a wide range of applications. Scaling up SCS is one of the main limitations hindering the commercialization of this technology. This is because of the high exothermicity, where large amounts of heat are released for a short duration. The process is vigorous and spontaneous and must be carefully considered to avoid explosions. Another serious problem is the possible formation of hazardous gases such as NOx and CO, formed from incomplete combustion. The third is the handling of the generated nanoparticles that can toxic. So far, most SCS is carried out in an open reactor system. Doing the SCS in a closed system would be an ideal way to address these toxic and handling challenges, but not the exothermic heat release challenge. In this study, we are focusing on understanding the impact of carrying out SCS in a closed system related to the physical properties of the synthesized material and its temperature-pressure data generated during the synthesis. For that we use, pseudo-adiabatic calorimetry (Phi-TEC I) as a tool to conduct solution combustion chemistry under adiabatic conditions that provides highly accurate data acquisition of temperature-pressure for the rapid exothermic nature of the SCS. We study the synthesis of nickel nanoparticles with nickel nitrate hexahydrate (oxidizer) and glycine (fuel) as the initial precursors that are dissolved in the methanol as solvent. The effect of metal/fuel ratio, amount of reactive mixture, and type of fuel were studied under adiabatic conditions in the calorimetry and compared with the nanoparticles in an open batch experiment. The temperature-pressure data from these studies open a new direction on the industrial scale-up of SCS with a high degree of control over the process. This work is a necessary first step toward carrying out the SCS in a closed reactor system.

ACKNOWLEDGMENTS

This work was made possible by funding from the Qatar National Research Fund (QNRF) project no. PDRA7-0414-21006 and co-funding by Shell Global Solutions International B.V.

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Nitrogen-Doped Graphene and Application as electrocatalyst for Proton Exchange Membrane Fuel Cells

Adriana Marinoiu*
Institute for Cryogenics and Isotopic Technologies – ICSI, Ramnicu Valcea, Romania (Romania)
* adriana.marinoiu@icsi.ro

Abstract ID #NSS-0520

Nitrogen-doped graphene is recognized as one of the most promising catalyst since it has demonstrated to act as a metal-free electrode with a good electrocatalytic activity and long-term operation stability for oxygen reduction reaction in proton exchange membrane fuel cells (PEMFCs). Graphene oxide received a remarkable attention as a valuable class of graphene derivatives, due to its chemical stability, high conductivity and ability to form chemical bonds easily. A simple, scalable, single-step synthesis method for nitrogen-doped graphene oxide preparation is presented in this paper, starting from commercial graphene oxide, urea and reducing agents; the reactions were carried out in microwave field using various conditions. Electrochemical measurements towards ORR indicated that the presence of nitrogen-doped oxide can effectively enhance the electrocatalytic activity and stability for ORR making it a candidate for practical application for PEMFCs.

ACKNOWLEDGEMENTS

This work was carried out through the Nucleus Program, financed by the Ministry of Education and Research, Romania, project no. PN 23 15 01 03 and project number PN-III-P2-2.1-PED2021-0840 PED 695/2022.

Magnetic Field Induced Effect in the Surface Plasmon Resonance Band of Silver Nanoparticles

Roman Redko[1 *], Vitaliy Shvalagin[2], Grigorii Milenin[3], Svitlana Redko[3]
[1] *V. Lashkaryov Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine, State University of Telecommunications (Ukraine)*
[2] *L. Pysarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine (Ukraine)*
[3] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine (Ukraine)*
* redko.rom@gmail.com

Abstract ID #NSS-0526

Magnetic fields induced effects in chemical reactions have long been the subject of investigation and still remail actual [1, 2]. Therefore, the obtaining new information about magneto-induced phenomena will contribute to a better understanding of magneto-induced processes in nanostructures. The ethanol solutions of the ZnO nanoparticles were placed in a constant and homogeneous weak magnetic field (B = 60 mT). Exposure time in the field was: 1 hour, 1 day and 5 days. These solutions were used for photocatalytic formation of ZnO/Ag nanoheterostructures under the action of UV irradiation. The production cycle was repeated during 30 days. During this time, the evolution of the obtained optical absorption spectra of solutions containing ZnO/Ag nanoparticles were measured on a Specord 210 spectrophotometer (relative to a cuvette with pure ethanol), SEM TEM microscopy data. For reliability of the received results the solution which was not exposed in magnetic field, but stored together with all samples at the same temperature conditions was used as a reference. Under the UV action, photocatalytic reduction of Ag (I) and the formation of a ZnO/Ag colloidal heterostructure occurs, which is characterized by an absorption maximum at 400–460 nm. Moreover, increasing the UV dose leads to a long-wavelength displacement of this peak. These processes are characteristic for all studied samples. But the energy positions of the observed peaks of the surface plasmon resonance band of silver nanoparticles of low and maximum doses of weak magnetic field exposition do not match. That is, the longer exposition of the ZnO solution in the magnetic field results to more essensial shift of the plasmon absorption peak to the blue spectral region with respect to the reference sample. This dependence is estimated to be quasi-exponential. Since the peak of surface plasmon resonance band of nanoparticles related to dimension of the nanoparticles, one can think that magnetic field treatment of the ethanol solutions of the ZnO nanoparticles results in more smaller ZnO/Ag nanoheterostructures creation. This feature was confirmed by SEM and TEM measurements. It was found that within 30 days the final position of the maximum of plasmon absorption of the Ag nanoparticles, which were formed on ZnO solutions, that have been undergone magnetic field treatment, slowly shifts to the position of the latter in the reference sample. The latter circumstance could indicate a "memory effect" that lasts for a month. Possible mechanisms, which could be responsible for the observed features are discussed.

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Silver-Containing Nanocomposites with Antimicrobial and Antiviral Activity

Valeriy Demchenko[1*], Nataliya Rybalchenko[2], Tetiana Hnatiuk[2], Krystyna Naumenko[2], Svetlana Zahorodnia[2], Maksym Iurzhenko[3], Sergii Riabov[4]
[1] *Institute of Macromolecular Chemistry, NAS of Ukraine (Ukraine)*
[2] *D.K. Zabolotny Institute of Microbiology and Virology of the National Academy of Sciences of Ukraine (Ukraine)*
[3] *E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine (Ukraine)*
[4] *Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine (Ukraine)*
*dvaleriyl@ukr.net

Abstract ID #NSS-0528

Infectious diseases caused by viruses and microorganisms continue to be one of the health problems worldwide, despite the rapid progress in the creation of drugs and the development of pharmaceutical technologies.

Therefore, today there is a need for new materials with a higher antiviral and bactericidal effect, and less toxicity for humans and the environment (ecology, medicine, and the food industry).

In this work, silver-containing nanocomposites Na-CMC–Ag–chitosan of low, medium, and high molecular weight were synthesized by reducing silver ions in polyelectrolyte-metal complexes using ultraviolet irradiation of different wavelengths (λ = 254 nm and 365 nm) and by sputtering silver nanoparticles on the surface of polyelectrolyte complexes.

The reduction of silver ions to metal nanoparticles was monitored by XRD.

Using the method of transmission electron microscopy, it was established that during the reduction of silver ions by ultraviolet irradiation with a wavelength of λ = 254 nm, smaller nanoparticles are formed than at 365 nm. It was found that in samples Na-CMC–Ag–chitosan of low, medium, and high molecular weight, the size of nanoparticles increases with an increase in the molecular weight of the cationic polyelectrolyte. A layer of ~200 nm thick Ag particles is formed in nanocomposites Na-CMC–Ag–chitosan low molecular weight obtained by sputtering silver nanoparticles.

A tendency towards an increase in antimicrobial activity in samples based on Na-CMC and chitosan was established with a decrease in the molecular weight of chitosan in relation to the test cultures of microorganisms S. aureus, E. coli, P. aeruginosa, C. albicans. It was shown that samples of Na-CMC – Ag – chitosan of low molecular weight, obtained by ultraviolet irradiation of silver ions of a shorter wavelength, exhibit higher antimicrobial activity against the microorganisms under study.

Antiviral activity of the created silver-containing nanocomposites against influenza A virus and herpes simplex virus 1 was revealed.

Cytotoxicity studies of nanocomposites on two cell lines MDCK and BHK show that the obtained samples are non-toxic.

Design and Structural Characterization of Semiconducting ZnO/ZnS Hierarchical Nanostructures on the Surface of Porous Silicon

Yana Suchikova*, Sergii Kovachov, Ihor Bohdanov
Berdyansk State Pedagogical University (Ukraine)
* yanasuchikova@gmail.com

Abstract ID #NSS-0530

The development of solid-state electronics requires researchers to search for cutting-edge materials capable of ensuring the functionality and reliable operation of electronic devices. Today, the creation of advanced materials focusses on the synthesis of heterostructures and heterolayers, which allow the creation of various types of barriers in electronic devices, expanding their functional capabilities and application fields [1, 2]. The main problems in growing A2B6-based heterostructures arise due to significant lattice mismatch and thermal expansion coefficients of the constituent structures. Here, we report on the synthesis technology of hierarchical ZnO/ZnS nanostructures on the surface of porous silicon and the investigation of structural and morphological properties. The choice of ZnO and ZnS synthesis materials is due to the fact that these semiconductors have relatively good chemical stability, high catalytic efficiency, excellent electron mobility, and strong adsorption capacity. To form the hierarchical structures, a two-stage method was chosen. During the first stage, a suspension of high-purity ZnS powder was prepared, which was applied to the surface of por-Si using the spray pyrolysis method. Then, thermal annealing was conducted in an oxygen atmosphere at 500 ° C for two hours to obtain polycrystalline ZnO. The ZnO/ZnS heterojunction is characterised by charge carrier separation because of differences in the values of the bandgap widths (3.37 eV and 3.67 eV for ZnO and ZnS, respectively). Finally, ZnO reliably passivates the surface of ZnS, reducing device degradation during long-term operation in normal or aggressive environments. Further investigation of the properties of the synthesised heterojunction is required, as well as the establishment of dependencies on the nanoarchitecture of the surface.

ACKNOWLEDGMENTS

The study was supported by the Ministry of Education and Science of Ukraine, namely No. 0122U000129, No. 0121U10942, No. 0123U100110. Yana Suchikova thankful for the support from COST Action CA20129 MultIChem.

We also thank the Armed Forces of Ukraine for the safety to carry out this work. This work was only possible thanks to the resilience and courage of the Ukrainian Army.

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Low Density Polyethylene Composites Filled With Iron (III) Oxide/Carbon Nanotubes Hybrid Nanoparticles

Anastasiia Kobyliukh[1*], Karolina Olszowska[2], Yevgen Mamunya[3], Marcin Godzierz[4], Marta Musioł[5], Slawomira Pusz[2], Urszula Szeluga[2]

[1] *Center of Polymer and Carbon Materials, Polish Academy of Sciences; Institute of Macromolecular Chemistry, National Academy of Sciences of Ukraine (Ukraine)*

[2] *Centre of Polymer and Carbon Materials, Polish Academy of Sciences (Poland)*

[3] *Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine (Ukraine)*

[4] *Polish Academy of Sciences, Centre of Polymer and Carbon Materials, Curie-Skłodowskiej 34 street, 41-819 Zabrze (Poland)*

[5] *Centre of Polymer and Carbon Materials, Polish Academy of Sciences, Marie Curie-Sklodowskiej 34, 41-819 Zabrze, Poland (Poland)*

*akobyliukh@cmpw-pan.edu.pl

Abstract ID #NSS-0533

Conductive polymer composites (CPC) have atracted attention of the both academic and industrial communities due to their good mechanical properties, tunable electrical properties (10−8–106 S/m) and relatively low manufacturing cost. To create such polymer composites, different conductive fillers, such as metal or carbon particles were incorporated into electrically insulating matrix [1]. The key properties of the obtained CPCs are strongly dependent on the filler structure i.a. size and shape of filler particles, their content in polymer matrix and specific polymer-filler inteactions. Recently, an increasing number of studies draws attention to the hybrid fillers, like metal-carbon, metal-metal, carbon-carbon [2], that can significantly improve magnetic, thermal and electrical properties of the final product. Fillers able to be oriented under the external magnetic field allow for considerable improvement in the electrical and thermal conductivities of final polymer composites [3,4].

The aim of this study was to characterize the structure and basic properties of multifunctional LDPE composites with a hybrid filler based on multi-walled carbon nanotubes (MWCNTs) coated with iron (III) oxide nanoparticles (IO NPs). The filler structure was confirmed by X-ray diffraction (XRD), Raman spectroscopy and scanning and transmission electron microscopies (SEM-EDS, TEM). LDPE composites with random and partially arranged distribution of filler NPs were prepared. Partial ordering of filler NPs in LDPE matrix using external magnetic field was confirmed by increased area ratio of D band to G band in Raman spectra of graphene layers. XRD and differential scanning calorimetry (DSC) were used to determine the effect of magnetic field and content of filler on the crystallinity degree of LDPE matrix. The crystallinity clearly increased for 5 vol.% and continued to rise up for 10 vol.% of filler loading applied in magnetic field. The effect of filler content and magnetic treatment on thermal and electrical properties of LDPE composites was studied in relation to the possibility of application them as electrically conductive polymer composites for piezoresistive sensors.

ACKNOWLEDGMENTS

This work was partially realized in the frame of:

- Polish-Ukrainian Research Laboratory ADPOLCOM "Formation and characterization of advanced polymers and polymer composites" between the Polish Academy of Sciences and the National Academy of Sciences of Ukraine
- Bilateral project "Polymer nanocomposites with hybrid nanofillers for high-tech EMI shielding and piezoresistive materials" between the Polish Academy of Sciences and the National Academy of Sciences of Ukraine (2022-2024).

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Synthesis of Gold Nanoparticles by Sonogalvanic Replacement in Sodium Polyacrylate Solutions

Artur Mazur*, Mariana Shepida, Galyna Zozulya, Orest Kuntyi
Lviv Polytechnic National University (Ukraine)
*mazurartur96@gmail.com
Abstract ID #NSS-0546

The unique optoelectronic properties of gold nanoparticles predetermine a wide range of applications in high-tech fields, such as sensory probes, photovoltaics, drug delivery therapeutic agents, catalysis, and electronic conductors [1]. The functional properties of AuNPs depend on the shape, size, and aggregate state, so choosing their synthesis method is essential. Sonogalvanic replacement in surfactant solutions ensures the controlled synthesis of stabilized metal nanoparticles in the solution volume [2, 3]. Ultrasound increases the sacrificial metal dissolution rate due to the intensive renewal of anodic areas. As a result, ion recovery is accelerated, contributing to metal nanoparticle nucleation and formation. Surface-active substances due to adsorption and formation of surface complexes with nanoparticles, suppress their growth during galvanic replacement and prevent agglomeration in solutions. Thus, it is possible to obtain metal nanoparticles with a small average size (up to 20 nm) and distribution range. This work established the regularities of controlled synthesis of gold nanoparticles by galvanic replacement of aurum ions with magnesium in sodium polyacrylate solutions in an ultrasonic field. In the investigated range of concentrations of HAuCl4, NaPA, and temperatures at US power of 20 W and frequency of 20 kHz, solutions of stabilized AgNPs have formed with an absorption maximum at ~530...540 nm, which corresponds to the size of AuNPs 10...40 nm. Considering the non-toxicity of polyacrylate and magnesium ions and their low price, such studies are relevant in creating the foundations of "green" technologies of metal nanoparticles.

ACKNOWLEDGMENTS

This work was carried out with the partial financial support of the National Research Founda-tion of Ukraine. Project registration number: 2020.02/0309 ("Design of polyfunctional nanostructured mono- and bimetals with electrocatalytic and antimicrobial properties").

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The Nanostructured NiFeCrWMo High-Entropy Alloy Binder versus Traditional Co Binder for WC-based Hard Alloys

Serhii Nakonechnyi*, Alexandra Yurkova
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)
*sergeynuts@gmail.com

Abstract ID #NSS-0566

The use of nanostructured and nanosized binders in the production of hard alloys is one of the most promising methods for improving their properties [1]. The nanostructure and nanosize of the binder particles provides high mechanical properties (hardness, strength, fracture toughness), high activity during sintering, etc [2,3]. In addition, the use of various alloys and advanced materials such as high-entropy alloys as nanostructured and nanosized binders allows to improve various characteristics of hard alloys in both normal and extreme operating conditions [3,4]. However, this raises a significant challenge to preserve the nanostructured state or particle size and, consequently, to obtain the desired characteristics of the resulting material.

In this work, two hard alloy systems with a nanostructured NiFeCrWMo high-entropy alloy and nanosized Co as binders, respectively, were obtained by electron beam sintering. X-ray diffraction and microstructural analyses revealed that the nanostructured NiFeCrWMo high-entropy alloy, due to the effect of "sluggish diffusion" and the content of refractory elements, significantly inhibits both the growth of WC grains and its own grain structure, forming thin layers of ~200-300 nm around WC particles without agglomerations of binder particles, pores, or their diffusion into carbide phases. At the same time, the hardness (93 HRa vs. 89 HRA for the Co binder) and fracture toughness (11.4 MPa·m1/2 vs. 9.5 MPa·m1/2 for the cobalt binder) characteristics reflect a significant positive effect of using the nanostructured NiFeCrWMo high-entropy alloy as a binder. Thus, this result opens broad prospects for the further production of these hard alloys with significantly improved characteristics.

This study represents first step to develop hard alloys of given composition for various purposes and characteristics by grinding WC grains, changing the binder content, etc. In addition, it is advisable to further investigate the effect of changing the elemental composition of a high-entropy binder and a variety of traditional and new methods of obtaining/sintering.

ACKNOWLEDGMENTS

This study was funded under the project of the Ministry of Education and Science of Ukraine, state registration number 0121U109789.

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Electrochemical Fabrication of Poly(6-aminoindole) – Graphene Oxide Nanostructures on Transparent Electrodes

Yuliia Horbenko*, Olena Aksimentyeva, Vasyl Kordan
Ivan Franko National University of Lviv (Ukraine)
*Yuliia.Horbenko@lnu.edu.ua

Abstract ID #NSS-0572

The nanochemistry, sensor, and organic electronics development leads to a constant search for easier-to-synthesize, cheaper polymer composite materials with new physicochemical properties. Materials based on the heteroaromatic compounds containing an aromatic ring (conjugated system) and a nitrogen atom are arousing the intense interest of researchers since the electronic properties of conjugated polymers are similar to those of inorganic semiconductors. Polyaminoindole (PAIn), among the substances of this class, has a relatively high electrical conductivity, good thermal stability, and a slower rate of degradation compared to other conducting polymers [1]. Surfaces covered with a thin layer of polyaminoindole exhibit catalytic properties during the electrooxidation of organic substances, are stable in aqueous solutions, and inhibit corrosion due to the good adhesion of the polymer film to the metal surface [2]. Composite materials based on PAIn are used in the electrochemical immunosensors with ultrahigh sensitivity manufacturing [3] and lithium-ion rechargeable batteries [4]. It was reported that poly(6-aminoindole) surface films at gold show reversible redox activity accompanied by color changes [5]. However, the electrochemical deposition of this indole derivative, especially in the presence of doping components, needs to be studied and improved. In this work, we investigated the influence of graphene oxide (GO) on the conditions of electrochemical polymerization of 6-aminoindole, the features of the polymer chain structure.

Poly(6-aminoindole) films were obtained on flexible optically transparent substrates of polyethylene terephthalate covered with a thin conductive layer of indium-tin oxide (PET-ITO). Polymerization was carried out by potential sweep mode in acidic media. It was established that monomer electrooxidation takes place in the range of potentials of 0.6-0.8 V vs. Ag/AgCl and leads to the formation of uniform polymeric films. According to IR spectroscopy, the polymerization of 6-aminoindole occurs due to the formation of a C-N bond in the 1,3 positions along the molecule chain, while the amino-group does not participate in the joining process. The electrochemical behavior of PAIn doped with GO was studied in the range of potentials E = -0.9... + 1.0 V. The possibility of catalytic electrooxidation of reduced GO on the PAIn film was revealed. The SEM images of poly(6-aminoindole) films obtained in the presence of GO clearly show very different morphologies with dissimilar particle sizes compared to the unmodified PAIn film. The ordered grid formation of GO uniformly distributed over the film surface is observed. In addition, with an increase in the potential sweep, the PAIn/GO interfacial boundary becomes thinner.

ACKNOWLEDGMENTS

This work was partly supported by the Simons Foundation (Award Number: 1037973).

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Dissolution-Precipitation Synthesis, Structural and Biological properties of Copper Whitlockite

Aleksej Zarkov[1*], Diana Griesiute[1], Agne Kizalaite[2], Vytautas Klimavičius[3], Arita Dubnika[4], Tomoyo Goto[5], Tohru Sekino[5]

[1] *Institute of Chemistry, Vilnius University, Naugarduko g. 24, LT-03225, Vilnius, Lithuania (Lithuania)*
[2] *Vilnius University (Lithuania)*
[3] *Institute of Chemical Physics, Vilnius University, Sauletekio 3, LT-10257, Vilnius, Lithuania (Lithuania)*
[4] *Riga Technical University (Latvia)*
[5] *Osaka University (Japan)*

* aleksej.zarkov@chf.vu.lt
Abstract ID #NSS-0573

Calcium phosphates (CPs) are major inorganic constituents of human hard tissues. This reason makes synthetic CPs widely used in the fields of bone regeneration and dentistry. Despite the fact that magnesium whitlockite ($Ca_{18}Mg_2(HPO_4)_2(PO_4)_{12}$) is the second most abundant mineral in human body, synthetic whitlockite is not so frequently used in practice. One of the reasons is that its preparation is challenging and synthesis products often contain impurities. On the other hand, whitlockite is biocompatible, have excellent osteogenic properties and it is more stable in acidic conditions than other CPs. These properties make whitlockite a promising candidate for the use in damaged bone regeneration or dental application [1].

Although the first row transition metal ions are of comparable size with Mg^{2+} ions, there are just several studies on materials with whitlockite structure, where Mg is replaced by other divalent cation [2-5]. At the same time TM ions can provide some very specific properties. Currently, there is an enormous interest in Cu-containing CPs due to bio-functional advantages offered by Cu such as antibacterial, angiogenic and osteogenic properties.

In this work, new calcium phosphate copper whitlockite ($Ca_{18}Cu_2(HPO_4)_2(PO_4)_{12}$, Cu-WH) was synthesized and comprehensively characterized. The synthesis of powders was performed by dissolution-precipitation method in aqueous medium under hydrothermal conditions. Phase conversion from brushite ($CaHPO_4 \cdot H2O$) to Cu-WH took place in acidic medium in the presence of Cu^{2+} ions. Optimization of synthesis conditions in terms of medium pH, temperature, time, Ca-to-Cu molar ratio and concentration of starting materials was performed. It was demonstrated that phase transformation occurs in a very narrow pH range (6.4-6.5), the formation of neighboring crystal phases was observed at different pH values. The study on thermal stability revealed that synthesized compound is thermally unstable and at higher temperatures decomposes to β-tricalcium phosphate and calcium pyrophosphate, analogically as biomineral magnesium whitlockite. The crystal structure of synthesized products was confirmed by XRD, FTIR and Raman spectroscopies, solid state NMR and EPR. Morphological features and elemental distribution within synthesized powders were studied by means of SEM/EDX analysis. The ion release in SBF solution was estimated using ICP-OES. Cytotoxicity experiments were performed with MC3T3-E1 cells.

ACKNOWLEDGMENTS

This research was funded by a grant WHITCERAM (No. S-LJB-22-1) from the Research Council of Lithuania.

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Direct Atomic Layer Processing on Complex Surface Morphologies

Maksym Plakhotnyuk[1*], Atilla Varga[2], Karolis Parfeniukas[2], Ivan Kundrata[1], Julien Bachmann[3]
[1] *ATLANT 3D Nanosystems, Kongens Lyngby (Denmark)*
[2] *ATLANT 3D Nanosystems, Taastrup, Denmark (Denmark)*
[3] *Friedrich-Alexander Universität Erlangen-Nürnberg (Germany)*
*mp@atlant3d.com

Abstract ID #NSS-0578

Unlike Atomic Layer Deposition (ALD), conventional vapor phase deposition techniques such as Physical Vapor Deposition (PVD) and Chemical Vapor Deposition (CVD) are limited by line of sight, which does not allow for conformal coating of complex surfaces. ALD, however, lacks the ability to selectively deposit material in a given region hence, ALD is often combined with other techniques, such as lithography, to create patterns and/or masks for area selective deposition. This can be a very time-consuming and costly process which usually includes 6 steps from film deposition to resist strip.[1] Atomic layer advanced/additive manufacturing can alleviate these issues while providing flexibility both in materials and device geometry.[2-4] Here we demonstrate ATLANT 3D technology provides the first-ever on-demand atomic layer advanced manufacturing technology based on hybrid Microreactor Direct Atomic Layer Processing (µDALP™).[5] Films deposited with µDALP™ have conformal coverage of gratings, microchannels and trenches up to a depth of 25 µm using a Platinum deposition process (Fig. 1). Substrates with a surface roughness including Carbon nanograss (Fig. 2), black silicon and anodized Aluminum Oxide membranes were also conformally coated with roughness up to an aspect ratio of 1:25 again with Platinum and TiO2. Our results demonstrate how a given ALD material process (in this case, Pt and TiO_2) can be used with ATLANT 3D technology to deposit localized area conformal coatings of complex surfaces with an aspect ratio of 1:25. The µDALP™ technology enables rapid prototyping and manufacturing for an array of applications from sensors (temperature, pressure, gas sensing and capacitive) to optics, all with sensitivities that meet or exceed those of devices made using conventional vapor phase deposition techniques.5 In addition, rapid localized processing facilitated by ATLANT 3D technology of such devices enables design innovation and optimization not possible with other thin film deposition techniques and lithography.

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Structure, Optical Properties and Photocatalytic Activity of Undoped, Y_2O_3-Doped ZnO Nanocomposites

Olga Chudinovych[1*], Denys Myroniuk[1], Liliia Myroniuk[1], Ihor Danylenko[2]
[1] *Frantsevich Institute for Problems of Materials Science, NAS of Ukraine (Ukraine)*
[2] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine (Ukraine)*
*chudinovych_olia@ukr.net

Abstract ID #NSS-0594

Zinc oxide is an important material due to its optical, photocatalytic, and magnetic properties. Doping ZnO with Y^{3+} ions increases its photocatalytic activity, helps create transparent coatings displays, improves UV radiation in photoluminescence (PL), etc [1].

The undoped and Y_2O_3-doped ZnO nanocomposites were obtained by the Pechini method. Solutions of Zn^{2+} and Y^{3+} nitrates, which were obtained by dissolving zinc and yttrium oxides with a content of the main component of 99.99% in nitric acid, were used as starting materials. Before preparing the initial solutions, yttrium oxide was pre-dried in a muffle at 300 °C for 2 hours. A mixture with different Y^{3+} content was prepared from nitrate solutions. The samples were subjected to X-ray powder diffraction using a DRON-3 diffractometer at room temperature (Cu-Ka radiation). The scan angle was 0.05–0.1 ° in the range 2q = 15–80 °. The undoped ZnO nanoparticles are identified as a wurtzite structure ZnO. For all Y2O3-doped ZnO samples, the diffraction peaks are almost similar to undoped ZnO. The XRD patterns of the Y_2O_3-doped ZnO do not show any other peaks corresponding to Y, Y_2O_3 or any other additional phases associated with impurities.

According to SEM, the synthesized powders have a conglomerate structure.

Micro-Raman scattering measurements were carried out to study the influence of Y^{3+} doping on the structural and vibrational properties of ZnO samples.

Photocatalytic activities of undoped and doped with 1, 2, 3, 4, 5 and 10 % yttrium oxide ZnO nanopowders were studied by the decomposition of aqueous methyl orange (MO) dye solution.

ACKNOWLEDGMENTS

This work supported by the research project of the NAS of Ukraine "Creation of promising materials based on ZnO doped REE for use in catalysis".

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Fabrication and Application of Meso-Porous Activated Carbon @ZSM-5 Composite Derived from Coal Gasification Slag and Fly Ash for the Adsorptive Removal of Pharmaceuticals in Aqueous Media

Xoliswa Cingo[1*], Odwa Mapazi[2], Luthando Nyaba[3, 4], Philiswa Nosizo Nomngongo[3, 4]
[1] *University of Johannesburg (South Africa)*
[2] *Analytical chemistry division, Mintek (South Africa)*
[3] *Department of Chemical Sciences, University of Johannesburg, Doornfontein, Johannesburg 2028 (South Africa)*
[4] *Department of Science and Innovation-National Research Foundation South African Research Chairs Initiative (DSI-NRF SARChI) in Nanotechnology for Water, University of Johannesburg, Doornfontein, Johannesburg 2028 (South Africa)*

*Xoliswacing@gmail.com
Abstract ID #NSS-0595

Increasing the application of precious elements present in coal fly ash and coal gasification slag is of great importance for waste management, recovery, and the preservation of the environment due to the large annual emission of this coal waste. The mixture of inorganic minerals and unburnt carbon hinder the use of coal waste, hence there is a necessity to separate the ash materials and unburnt carbon for resource utilization of coal gasification slag and fly ash. This study successfully prepared a nanostructured composite composed of mesoporous activated carbon and zeolite-Socony mobil-5 (AC@ZSM-5) generated from coal gasification fine slag and coal fly ash through carbothermal treatment, chemical treatment, and hydrothermal treatment. The synthesized material was applied for the enrichment of non-steroidal anti-inflammatory drugs in wastewater. The most significant parameters affecting the extraction procedure were optimized using response surface methodology based on central composite design. Under optimum conditions the method exhibited relatively low limit of detection and quantification and relative standard deviation. Three selected pharmaceutical compounds such as aspirin, paracetamol and ibuprofen were successfully extracted and quantified using high performance liquid chromatography equipped with a photodiode array detector (HPLC-DAD). The sorbent was characterized using high resolution scanning microscopy (HR-SEM), transmission electron scanning microscopy (TEM), N2 adsorption/desorption isotherms, X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), thermogravimetric analyser (TGA) and zetapotential. The techniques confirmed that the prepared material had high surface area, highly porous and offers strong binding affinity for target analytes. The AC@ZSM-5 composite showed excellent adsorption properties towards the three-target analytes with remarkable adsorption capacity. The sorbent selectively removed all the target compounds in real water samples. The sorbent could be reused several times with little loss in extraction efficiency.

ACKNOWLEDGMENTS

This work was supported by the University of Johannesburg and Mintek.

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Photodynamics of Temperature Tuned Dual Colour Emission in Mn-Doped ZnS-CdSe Janus Coupled Quantum Dot

Vivek Chaudhary*, Sri Sivakumar
Indian Institute of Technology Kanpur (India)
* vivekch@iitk.ac.in

Abstract ID #NSS-0597

Coupled Quantum dots (CQDs) formed using individual quantum dots gives an extraordinary application ranging from optoelectronics, quantum information processing to biolabeling. CQDs with three different morphologies named Acorn, Janus, and core-shell have been formed by varying the precursor ratios of Cd to Zn using ZnS and CdSe as individual Quantum Dots.

Manganese (Mn) is a well-known transition metal dopant for modifying the optical characteristics of host semiconductor nanocrystals (NCs). In the present work, we have formed Mn-doped ZnS-CdSe coupled quantum dot to study energy transfer as function of host band gap and spin orbit coupling for the first time to best of our knowledge. Mn^{2+} doped ZnS QDs revealed intense photoluminescence 4T1(4G) – 6A1(6S) transition while in Mn^{2+} doped CdSe does not show any significant peak at 2.12eV. This quenching of 2.12eV photoluminescent peak led us revisit the problem and understand dynamics of dopant with host nanocrystal. We elucidate quenching of Mn-dopant strong photoluminescence peak 2.12eV at room temperature and temperature below sub-zero level (upto 80K). It is plausible to see the presence of a characteristic dopant emission peak as well as a longer lifetime when the temperature is lowered, implying that both band gap and composition influence Mn emission. Although this emission is assumed to be atomic like in origin, recent literature has discovered many dependencies on the host NCs that permit energy/charge transfer to a spin and orbital prohibited channel. Decay lifetime for the Mn^{2+} doped CQD revealed that the decrease in decay lifetime with doping. The quantum yield for Mn^{2+} doped CQD photoluminescence is nearly 37% which decays over a few nanoseconds.

The Eco-Friendly Method Synthesis of MXenes Materials Using Surface Acoustic Wave

Joanna Sulej-Chojnacka[1*], Joanna Półrolniczak[2], Grzegorz Kubicki[1], Ernest Brzozowski[3]
[1] *Łukasiewicz Research Network—Pozna´n Institute of Technology, 6 Ewarysta Estkowskiego St., 61-755 Poznan (Poland)*
[2] *Łukasiewicz Research Network—Pozna´n Institute of Technology, 6 Ewarysta Estkowskiego St., 61-755 Poznan. (Poland)*
[3] *Łukasiewicz Research Network–Institute of Microelectronics and Photonics, Warsaw, Poland (Poland)*
* joanna.sulej-chojnacka@pit.lukasiewicz.gov.pl
Abstract ID #NSS-0607

Over the last decade, two-dimensional materials have gained importance, which exhibits properties drastically different from their precursors, i.e. 3D materials. MXene is a relatively new member of the 2D material group, but this group has become a key material in modern times [1,2].

These materials are typically synthesized by time-consuming and labor-intensive multi-step procedures involving chemical etching and exfoliation of atomically laminated parent materials. Conventional synthesis methods use aggressive reagents that can cause defects and can lead to the destruction of MXenes and the formation of carbide-derived carbon [3].

In our research, we demonstrate a one-step and ultra-fast SAW synthesis method. Surface Acoustic Wave (SAW) technology is not new and is heavily used in many industrial fields, such as telecommunications gas sensors and electrical circuits, signal filtration, flow measurement, microfluidics, and in the field of material synthesis, e.g. two-dimensional (2D) materials [4-6].

High purity MAX phases (Ti_3AlC_2 and Cr_2AlC) were the precursors of MXenes, and are produced by Authors by HEMB-SPS approaches. It used a low concentration of LiF solution and milliseconds to produce MXenes, compared to the HF etching technique, which requires concentrated corrosive and harmful liquid and long etching periods (at least 24h). The replacement of HF with low-cost, non-toxic fluoride salts (such as NaF, KF, and LiF) significantly reduces the environmental impact of the process.

The produced MXene was confirmed by XRD and SEM. Mainly, was proved the existence of individual MXene sheets dispersed in water.

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Fullerene $C_{60}@\{H_2O\}_n$: Obtaining Stable Aqueous Solutions Using Cryogenic Sublimation

Razet Basnukaeva*, Alexandr Dolbin, Mykola Vinnikov
B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine (Ukraine)

*razeta9556@gmail.com

Abstract ID #NSS-0612

Fullerenes are a molecular allotropic form of carbon having a spherical structure. C60 is the most extensively studied and well-known fullerene, which is made up of 60 carbon atoms arranged in a structure consisting of hexagons and pentagons. Complex compounds of fullerenes with water and other solvents were studied in [1, 2] and find applications in various fields. These complexes may have interesting physical and chemical properties, such as the ability to catalyze reactions, photoluminescent and antioxidant properties. A solid state of the $C_{60}@\{H_2O\}$ mixture was achieved by joint condensation of water vapor and fullerene C60 on a cooled substrate. Upon heating at room temperature and then melting, the mixture $C_{60}@\{H_2O\}$ forms a stable solution without the applying for additional treatment such as shaking or sonication. The cryogenic-sublimation technique was used to obtain aqueous colloidal solutions of $C_{60}@\{H_2O\}_n$ fullerene, which were then subjected to optical characterization studie (absorption spectroscopy, Raman spectroscopy) [1]. Additionally, comparative analysis of C_{60} fullerene films was performed using transmission electron microscopy and UV-visible range absorption spectroscopy. The films were obtained through two methods — vacuum deposition on a sapphire substrate and vacuum drying of an aqueous colloidal C_{60} solution at room temperature. The research findings indicated that the solutions under study primarily consisted of individual C_{60} molecules and small clusters, with a size of up to 10 nm. The study also revealed that C_{60} films, which were produced by drying an aqueous colloid solution of C_{60} in vacuum at room temperature, contain a significant amount of bound molecular water. These findings have potential applications in the development of membranotropic medicines, biologically-active substances, and other related fields.

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Morphological, Structural and Optical Changes of 2D ZnO Nanostructures Upon Addition of Sodium Nitrate ($NaNO_3$)

Asma Tadji*, Mokhtar Zerdali, Saad Hamzaoui
University of Sciences and Technology of Oran Mohamed Boudiaf Laboratory of Electronic Microscopy and Material Sciences – LEMMS- Oran, Algeria (Algeria)
* tadjiasma@yahoo.fr

Abstract ID #NSS-0615

Due to its interesting physical and chemical properties, 2D ZnO is considered one of the attractive semiconductors for nanoelectronic applications. In this study, 2D ZnO nanostructures are synthesized by hydrothermal method on a seeded glass substrate. The effect of adding sodium nitrate ($NaNO_3$) was studied. AFM images indicated that the two samples showed a growth of 2D ZnO nanostructures which exhibit the highest surface-to-volume ratio and specific facet (0001). The 2D ZnO nanostructures grown without $NaNO_3$ had a nanodiscs shape, with an average diameter of 174 nm and a thickness of about 46 nm. The addition of $NaNO_3$ results in much larger hexagonal nanosheets with an average diameter of about 290 nm and a thickness of about 2.2 nm.

Removal of Selected Recalcitrant β-Blocker in Water Systems by Adsorption Technology Combined with Advanced Oxidation Processes

Ngwako Joseas Waleng[1*], Philiswa Nosizo Nomngongo[2, 3]
[1] *University of Johannesburg (South Africa)*
[2] *Department of Chemical Sciences, University of Johannesburg, Doornfontein, Johannesburg 2028 (South Africa)*
[3] *Department of Science and Innovation-National Research Foundation South African Research Chairs Initiative (DSI-NRF SARChI) in Nanotechnology for Water, University of Johannesburg, Doornfontein, Johannesburg 2028 (South Africa)*
* ngwakowaleng@gmail.com

Abstract ID #NSS-0625

With the rapid advances in industries and agricultural practices, various toxic pollutants have been released into the aquatic environment over the past few decades. Pharmaceuticals among others, have been detected at concentrations which threaten the well-being of humans and ecological balance [1]. In this work, Fe_3O_4@NH_2-MIL-101(Cr) nanocomposite was successfully synthesized through facile in-situ chemical co-precipitation method. The prepared nanocomposite was characterized using Fourier transform infrared spectroscopy (FTIR), Ultraviolet-Visible spectroscopy (UV-Vis), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), transmission electron microscopy (TEM), x-ray diffraction (XRD), Brunauer-Emmett-Teller (BET), Photoluminiscence (PL) and electrochemical impedance spectroscopy (EIS) [2], [3]. The photocatalytic performance of the nanocomposite was evaluated by degradation of the selected β-blocker acebutolol (ACE) under visible light illumination provided by SynLED parallel photoreactor. Factors deemed to be affecting photodegradation process were optimized and these include mass of adsorbent (MA), pH, adsorption time (AT), analyte concentration and volume of the oxidant. The results indicated that the nanocomposite exhibited excellent photocatalytic activity for the degradation of ACE. Photoluminescence and EIS results showed that the incorporation of Fe3O4 nanoparticles into NH2-MIL-101(Cr) improved charge separation and transfer, which subsequently enhanced photodegradation efficiency [4], [5].

ACKNOWLEDGMENTS

FUNDING The authors are grateful for the financial assistance provided by Department of Science and Innovation-National Research Foundation-South African Research Chair Initiative (DSI-NRF SARChI) programme, grant number 91230 and National Research Foundation (NRF, South Africa, grant no:121638).

ACKNOWLEDGEMENTS The authors extended their gratitude to the University of Johannesburg (Chemical Sciences department) for providing us with their laboratory facilities for conducting our experiments. The gratitude is further extended to Mrs Orienda Sebabi Molahlegi and Mr Siyasanga Mpelane for their assistance in characterization techniques.

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Uniaxial Stress-driven Reconstructed Si (110)-"16×2" Surfaces

Hidehito Asaoka*
Advanced Science Research Center, Japan Atomic Energy Agency (Japan)
* asaoka.hidehito@jaea.go.jp

Abstract ID #NSS-0631

Tuning of surface stress is a powerful strategy for tailoring self-assembled nanostructures at the atomic scale. The ability to alter the stress (its magnitude, direction, extent, periodicity, and symmetry) allows versatile bottom-up construction. Silicon surfaces produce unique stress distribution corresponding to the reconstruction based on dangling bond reduction and adatom formation. It is known that a reconstructed Si(110)-"16×2" surface has a chiral structure (L or R) with one-dimensional mono-atomic steps and pentagon pair rows along [1-12] and/or [-112] directions. The chiral structures are generated as a double domain on the surface as well as a combination of both, however, no method has yet been established to reproducibly and selectively control the chirality of one of them. Here we show that an externally uniaxial stress-driven Si(110)-"16×2" structure controls the chiral one-dimensional reconstruction. We found the Si(110)-"16×2" reconstruction has anisotropic tensile stress intrinsically on the bulk Si(110)-1×1 structure. The anisotropic Si(110)-"16×2" structure has the potential to be tailored to self-assembled nanostructures by using uniaxial extrinsic stress. Furthermore, as expected, we were able to find selectively the chiral reconstructed structure. Our results demonstrate how to form homochirality on the Si surface, which consists of a one-dimensional chiral structure. We anticipate our results to be starting point for the establishment of a new highly efficient and stable method for the complete separation of chiral substances. It is also expected to have a significant ripple effect that will directly lead to innovations in novel optical silicon devices.

Design and Structural Investigation of $CuIn(Ga)Se_2$ Films for Solar Energy Applications

Sergii Kovachov*, Ihor Bohdanov, Natalia Tsybuliak, Hanna Lopatina, Anastasiia Popova, Yana Suchikova
Berdyansk State Pedagogical University (Ukraine)
* essfero@gmail.com

Abstract ID #NSS-0632

Semiconductor materials based on gallium and indium have gained popularity in recent years because of their wide use in solar energy. In particular, copper indium (gallium) diselenide (CIS), CuIn(Ga)Se2, has become an important semiconductor for the production of thin-film solar cells [1, 2]. The main methods for synthesising $CuIn(Ga)Se_2$ are magnetron sputtering, evaporation, and deposition. However, these methods require high processing temperatures and the use of high-tech equipment, resulting in high-synthesis-technology costs.

In this work, we propose a simple and cost-effective method for synthesising polycrystalline $CuIn(Ga)Se_2$ films, namely, liquid phase spray deposition. Using this method, a dense layer of $CuIn(Ga)Se_2$ with a granular structure was obtained. EDX analysis showed that indium and gallium are present in a 2:3 ratio, respectively. These data are well correlated with the results of XRD analysis. A Raman scattering study showed the absence of peaks of the Cu_2Se secondary phases. This indicates the effectiveness of the proposed synthesis technique and the prospects for its use on an industrial scale. These findings could lead to the development of more efficient and cost-effective solar cells based on $CuIn(Ga)Se_2$ films.

ACKNOWLEDGMENTS

The study was supported by the Ministry of Education and Science of Ukraine, namely No. 0122U000129, No. 0121U10942, No. 0123U100110. Yana Suchikova thankful for the support from COST Action CA20129 MultIChem.

We also thank the Armed Forces of Ukraine for the safety to carry out this work. This work was only possible thanks to the resilience and courage of the Ukrainian Army.

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Thermal Properties of Sulfur-Doped Graphene Oxide

Rashad G. Abaszade*
Azerbaijan National Academy of Sciences (Azerbaijan)
* abaszada@gmail.com

Abstract ID #NSS-0636

The fact that graphene-based samples have different properties puts it in the spotlight as promising materials. The unique optical and kinetic properties of carbon-based nanomaterials and nanocomposites have been very interesting [1-8] and are very important as new generation solar cells as well as important materials applied in optoelectronics. NTE results from the coupling between the resonances of planar material elements and phononvibrational modes [9], the coupling between acoustic and soft transverse optical phonons [10] and so on. At low temperature, NTE is intrinsic in 2D materials: transverse (out-of-plane) vibrational modes of interatomic bonds have lower excitation energy than longitudinal (in-plane) modes; at low temperatures despite an increase in the mean initial bond length with increasing temperature, their effective distance decreases due to the change in the bond angle caused by an increase in amplitude of the atom's transverse vibration [11]. The graphene oxide sample obtained by the Hammer method was studied by scanning electron microscopy, energy-dispersive X-ray spectroscopy, Raman spectroscopy, DSC and TEM methods. It was found that the addition of a sulfur source to graphene oxide multiplies its negative thermal expansion for two percent doped samples with a carbon to oxygen ratio of 2.3 in a certain room temperature range. It was found that the interaction between the layers enhances the negative thermal expansion. In contrast to graphene oxide, the as-grown sulfur-doped samples exhibit a nonlinear temperature dependence of thermal expansion. The negative thermal expansion is explained by the coupling between resonances of structural elements and phonon backscattering. Reducing the size of crystallites electrical, optical, thermal and mechanical properties (surface and space charges) dominated by their internal interface, and our findings suggest new possibilities for graphic materials in this respect.

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Green Colloidal Synthesis of MoS_2 Nanoplatelets

Filip Zechel[1*], Peter Hutár[1, 2], Viliam Vretenár[3], Karol Végsö[4], Peter Šiffalovič[5], Milan Sýkora[1]
[1] *Laboratory for Advanced Materials, Faculty of Natural Sciences, Comenius University, Ilkovičova 8, 84104 Bratislava (Slovakia)*
[2] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 841 04 Bratislava (Slovakia)*
[3] *Centre for Nanodiagnostics of Materials, Faculty of Materials Science and Technology, Slovak University of Technology, Vazovova 5, 812 43 Bratislava (Slovakia)*
[4] *Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 84511 Bratislava (Slovakia)*
[5] *Centre of Excellence for Advanced Materials Application, Dúbravská cesta 9, 84511 Bratislava (Slovakia)*
*zechel2@uniba.sk

Abstract ID #NSS-0647

2D materials are an intensely studied group of materials because of their remarkable size and shape dependent optical, electronic and mechanical properties.[1,2] MoS_2 is one of the most investigated 2D materials because of its unusual indirect-to-direct bandgap conversion upon transition from bulk to a single monolayer 2D structures.[3] The 2D MoS_2 is usually prepared by exfoliation from bulk structures,[4] or by Chemical Vapor Deposition (CVD) methods.[5] Recently it was reported that MoS_2 nanocrystallites can be also prepared by chemical methods of colloidal synthesis.[2] This approach gives a good control over the size and shape of the crystallites in the nanometer size range. However, most previously reported colloidal synthetical methods use toxic chemicals as starting materials. Here we report colloidal MoS_2 synthesis using low toxicity molybdenum and sulfur precursors. Six different compounds were examined as sulfur sources in combination with molybdenum acetate as the Mo source. The formation of MoS_2 crystallites was confirmed by HR-TEM imaging, EELS as well as by electronic absorption and Raman spectroscopies. Grazing Incidence Wide Angle X-ray Scattering (GIWAXS) and photoluminescence analysis of the products showed its polydisperse character in terms of lateral sizes. The effect of the precursors, solvent, and ligands on the kinetics of the crystal growth and the structure of the products will be discussed. Our results demonstrate the need for a broader investigation of reaction parameters influencing the growth of MoS_2 nanoplatelets and opportunities for a better control over the morphology of obtained nanocrystals using greener chemical approaches.

ACKNOWLEDGEMENTS

This work was supported by the European Union's Horizon 2020 research and innovation programme under Grant Agreement 810701, by the Slovak Research and Development Agency under Grant Agreement APVV-19-410 and Slovak Ministry of Education under grant agreement No. 1/0892/21.

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Researching of Biologically Active Polymeric Hydrogel Transdermal Nanomaterials Modification by Humic Acid

Katerina Lebedeva[1*], Anna Cherkashina[1], Tetyana Tykhomyrova[1], Victor Moiseev[1], Volodimir Lebedev[2], Andrij Masikevych[3]

[1] *National Technical University Kharkiv Polytechnic Institute (Ukraine)*
[2] *National Technical University «Kharkiv Polytechnic Institute» (Ukraine)*
[3] *Bucovin State Medical University (Ukraine)*

*oazis.ruk@gmail.com

Abstract ID #NSS-0653

Biologically active polymer hydrogel transdermal nanomaterials based on gelatin, sodium alginate, modified by humic acids, were designed and researched. Literature review was carried out and it was proved that humic acids using is perspective nanofiller for the functional effect on the biologically active polymer hydrogel transdermal properties. It has been found that effective processes for receiving biologically active polymer hydrogel transdermal nanomaterials based on gelatin, hydroxypropyl cellulose and sodium alginate can be carried out in different humic acids concentration values while achieving an increase in hydrogel polymers structuring processes. Humic acids modification in biologically active polymeric hydrogel transdermal nanomaterials based on gelatin and sodium alginate caused structure formation with high density, and resistance and with larger agglomerates in hydrogels. By carrying out rheological, conductometric and microscopic studies, it was found that the modification of gelatin-sodium alginate systems by humic acids allows receive receive biologically active polymeric hydrogel transdermal nanomaterials with higher swelling degree. The formation of a larger number of agglomerates in biologically active polymeric hydrogel transdermal nanomaterials based on gelatin and sodium alginate on the different content of humic acid is clearly visible from the microscopic studies results.It should be noted that the hydrogel delamination in biologically active polymeric hydrogel transdermal nanomaterials based on gelatin and sodium alginate on the different content of humic acid into the aqueous phase and the structured polymer phase does not occur. It is shown that the application of new biologically active polymeric hydrogel transdermal materials based on gelatin and sodium alginate modified by humic acids allows improving the skin moisture-lipid balance Modification of gelatin-based biopolymer hydrogels by humic acids makes it possible to obtain biologically active polymeric hydrogel transdermal nanomaterials with an increased swelling degree and ability to improve the skin moisture-lipid balance: from the initial moisture 34-36% and fatness 8-10%, they increase to 58-66% and 52-60%. In future researching is perspective to determine transdermal level of designed biologically active polymer hydrogels for most important medicine and cosmetic biologically active substances. So, designed polymer hydrogel based on gelatin, sodium alginate, modified by humic acids, are transdermal nanomaterials with good properties.

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Functionalization of Silica Particles with Polyisoprene or Methacrylate Groups to Improve Macroscopic Mechanical Properties of Thick Elastomeric Films

Olha Maikovych[1*], Emilie Choppe[2], Anna Stasiuk[1], Serhii Varvarenko[1], Wasan Thaokotsee[2], Jean-Francois Bardeau[2], Pamela Pasetto[2]
[1] *Lviv Polytechnic National University (Ukraine)*
[2] *Le Mans Université (France)*
*olha.v.maikovych@lpnu.ua

Abstract ID #NSS-0660

Silica particles, carbon black, sodium carbonate and so on are often used as fillers in elastomeric materials to enhance their mechanical properties, such as stiffness, strength, and toughness [1, 2]. However, the dispersion of particles in the elastomeric matrix is a challenging task, and agglomeration can occur. To overcome this problem, particles can be functionalized with polyisoprene or methacrylate groups.

Polyisoprene is a natural rubber polymer, which is similar to the elastomeric matrix. By functionalizing silica particles with polyisoprene, the interaction between the filler and the matrix can be improved. This can lead to better dispersion and stronger interfacial bonding, resulting in improved mechanical properties of the elastomeric material.

Thick elastomeric films are commonly used in various industrial applications, such as seals, gaskets, and coatings. The mechanical properties of these films are crucial to their performance, and the use of functionalized silica particles can improve their macroscopic mechanical properties.

In summary, functionalization of silica particles with polyisoprene or methacrylate groups can improve the macroscopic mechanical properties of thick elastomeric films.

In this preliminary study, silica particles were synthesized, and polyisoprene brushes were grafted. These functionalized particles were then inserted into thick elastomeric films and some mechanical properties were measured.

The key steps to obtain functionalized oligomers from natural rubber [3] (used for both silica functionalization and thick film synthesis) will be described as well as the general synthesis and characterization of hybrid particles and charged films obtained by photopolymerization of acrylic chains ends of the oligoisoprines.

A second type of particles were synthesized bearing simply a methacrylate group at the surface; this made them react with the cross-linker oligoisoprene used to prepare the film so that they remained covalently linked to the matrix. The influence of particle size and type of silica functionalization on the film physico-chemical properties will be discussed. Raman spectrometry was used for further characterization of silica and charged films. In addition, the use of chemometric analysis method made it possible to discriminate the films containing 1 % or 5 % weigh of functionalized particles with polyisoprene or methacrylate groups.

Conclusions

Initial results showed that the polyisoprene shell of silica particles made it easier to have a homogeneous dispersion in a polyisoprene cross-linked matrix than bare silica or silica particles functionalized with silica. The presence of core-shell particles increased mechanical properties such as tensile strength and elongation at break.

ACKNOWLEDGMENTS

This project has received funding through the MSCA4Ukraine project, which is funded by the European Union.

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Size Effect of Wetting of Amorphous Carbon by Micron Particles of Tin

Sergey Petrushenko[1*], Sergey Dukarov[2], Ruslan Sukhov[3], Sukhov Volodymyr[3], Mateusz Fijalkowski[4]
[1] *Technical University of Liberec, Institute for Nanomaterials; V.N. Karazin Kharkiv National University (Czech Republic)*
[2] *V. N. Karazin Kharkiv National University (Ukraine)*
[3] *V.N. Karazin Kharkiv National University (Ukraine)*
[4] *Technical University of Liberec, Institute for Nanomaterials (Czech Republic)*

*Serhii.Petrushenko@tul.cz

Abstract ID #NSS-0663

Wetting is the most important process parameter for systems in which solid and liquid phases come into contact. In applied research, wetting is of interest for soldering, impregnation of porous media, coating, ore enrichment, wastewater treatment, etc. In general scientific research, wetting patterns are necessary for understanding the interfacial interaction in contact pairs. In particular, the boundary wetting angle of a solid substrate melt determines the shape of islands formed during melting and the achievable magnitude of supercooling. The presence of a wetted surface also affects the magnitude of the size effect of melting and causes the capillary motion of the nanoparticles.

A peculiarity of the size effects of wetting is that it can be observed not only in nanostructures but also for micron-sized particles. Since nanoscopic and microscopic size effects are due to different mechanisms, the study of each of them is of some interest for the formation of a holistic scientific picture of wetting. Our work is devoted to the investigation of size effects of the wetting of carbon by microscopic particles formed during de-wetting of tin films.

Samples of the study were obtained by vacuum condensation. For this purpose, a thin film of carbon was deposited on the surface of a fresh chipped KCl monocrystal from a voltaic arc. Then a layer of tin was deposited on the thus amorphous substrate. After completion of condensation the obtained samples were heated above the melting point of the tin. Owing to the film substance melting and the accompanying processes of self-organization an island structure with approximately Gaussian size distribution appeared on the substrate surface. Thus, an array of particles of different sizes was formed on one sample. Due to this, the construction of the dimensional dependence was possible already on one sample. To determine the contact angle, chipping and slant observation methods were used, realized using a Tescan Vega3 LMH scanning electron microscope.

It was found that tin wets poorly amorphous carbon: the wetting edge angle for different particles is in the range 125-155°. Generally, for particles of the same size, the observed range of marginal angles is around 10°. This is considerably larger than the instrumental error of the measurement. Apparently, such a spread in the first approximation corresponds to the wetting hysteresis width and can be explained by substrate inhomogeneity and the kinetics of particle formation during solid film melting. It is shown that in the size range of 1-12 μm the contact angle increases linearly with increasing particle size. The observed dimensional dependence can be explained by the manifestation of linear contact line tension. The contact line tension estimated from the size dependence of the contact angle is 7.5 10-6 J/m

ACKNOWLEDGMENTS

This project has received funding through the MSCA4Ukraine project, which is funded by the European Union and also supported by the Ministry of Education and Science of Ukraine

Polymer Inorganic Nanocomposites for Electromagnetic Radiation Absorption Using Potassium Titanates

Serhii Kopylov[1*], Volodimir Lebedev[2], Maksym Riabchenko[1], Anna Cherkashina[1], Denis Miroshnichenko[2], Oleksii Shestopalov[1], Alina Hrubnik[1]
[1] *National Technical University Kharkiv Polytechnic Institute (Ukraine)*
[2] *National Technical University «Kharkiv Polytechnic Institute» (Ukraine)*
*moriabchenko@ukr.net

Abstract ID #NSS-0667

Scientific progress intensiveand technological development has led to avalanche-like decrease in the environment safety associated with have significantly increased electromagnetic pollution new sourcewith great costs to human health, safety, and the environment. This challenge is exacerbated by the appearance, of new sources of electromagnetic radiation and energy transmission such as cellular, satellite radio communication, navigation and radar systems, radio engineering installations, medical devices, household appliances and other technical equipment, intended for electromagnetic energy transmission and use [1]. The aim of the article isaims to studyinvestigate polymer inorganic nanocomposites for electromagnetic radiation absorption using potassium titanates. For the study polymer inorganic composites for electromagnetic radiation absorption, the following materials were used The selected polyamide 6 (durethane brand polyamide 6) and sodium polytitanates werepolytitanate nanomaterialsthat contain TiO_2, K_2CO_3 и KCl. It was sho. Sodium polytitanates nanomaterials were received by charge sintering that contain contains TiO_2, K_2CO_3 и KCl.K_2CO_3 and KCl. Ratio (in moles) TiO_2: K_2OK_2O was from 4:1 to 7:1 with the addition from the mass S TiO_2: K_2OK_2O 20 % wt. KClKCl. The charge is crushed, mixed, passed through a sieve of 60-300 microns and fired in the air in a muffle furnace for 1-3 hours at a temperature of 900 ° C (assumed product diameter is 0.005-0.1 microns and a length is 1-10 microns), then at 1000 °C (assumed product diameter 0.1-0.6 μm and length 5-60 μm), then at 1100 °C (assumed product diameter 0.6-2 μm and length 60-600 μm). The salt matrix (KCl) separation andfrom unreacted particles is carried outwas conducted by leaching with a slightly acidic solution with stirring or deionized water at a temperature of 90 °C,. It was then filtered, and the precipitate iswas washed until the chloride ion is completely removed. DryLastly, it was dried at 105-120 °C to a residual moisture content of 0.5-1% wt. Results showed that modification of polyamide 6 with sintering products in athe form of a fine nanopowder of potassium polytitanate that contain the primary phase $K_2O\times\times 2TiO_2$ with an admixture of a phase $K_2O\times\times 4TiO_2$ allows to increase, which increased their strength properties, while the. The modification of polyamide 6 with potassium polytitanate nanoparticles allows to increaseincreased their strength properties, while. It was also observed that the optimal content of silicon carbide is over 10 % by mass. At the same timeLikewise, it should be noticedwas observed that the overall effect of reinforcing potassium polytitanate nanoparticles effect was much worse than in reported in the literature [2], which is directly related]. This observation could be ascribed to the direct formation of an exclusively potassium polytitanate particles amorphous phase. In fact, based in the potassium polytitanate nanoparticles. The optimal content of potassium polytitanate was over 10 % by mass. To fully ensure the reinforcing effect due to the filling of potassium polytitanate polyamide 6, it is necessary to use whiskers $K_2O\times\times 6TiO_2$, which can be receivedcollected by the additional crystallization of the amorphous charge sintering product additional crystallization.

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DFT Computational and Experimental Studies of Cellulose Molecules Interaction with Carbon Nanostructures

Yuriy Hizhnyi[1], Tymur Isokov[1*], Viktor Borysiuk[1], Serhii Nedilko[1], Yaroslav Zhydachevskyy[2]
[1] *Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *Institute of Physics Polish Academy of Sciences (Poland)*
*isokovtd@gmail.com

Abstract ID #NSS-0669

Nanocomposites based on cellulose and carbon nanostructures (CNS) are studied as perspective multifunctional materials [1]. Despite intensive studies, some open questions regarding the peculiarities of the interaction of the components of nanocomposites "cellulose-CNS" still exist [2,3]. In particular, the questions regarding the types of bonds formed in the material between components, the mutual influence of the components on their physical (electronic, optical and other) properties, the role of individual components in formation of the materials properties remain unclear. The purpose of our work is to find some answers to these questions using theoretical (computational) research and comparison of their results with experimental data.

The contribution presents results of theoretical studies of the interaction of cellulose molecular clusters with carbon nanostructured materials: carbon nanotubes and graphene. The studies are carried out in the form of calculations of the electronic structure performed by the quantum chemical method in the DFT approximation [4]. The calculations revealed the mechanisms of adsorption of molecular cellulose on the surface of carbon nanotubes CNT(5,5) and single-layered graphene sheets, both bare and doped with boron or nitrogen. Binding energies and inter-nuclear distances between adsorption components are calculated and analyzed. The types of interatomic bonds between adsorbed cellulose molecules and carbon surfaces are elucidated.

It was found that adsorption of cellulose molecules on the surface of undoped CNTs should generally be considered unlikely, as calculations show the absence of covalent interatomic bonds. Interaction of cellulose molecules with graphene surface should be more pronounced if compared to the case of nanotube surface because the obtained interatomic distances between cellulose and graphene atoms are significantly shorter. In general, interaction of cellulose components with the surfaces of carbon components of composite materials should be considered as relatively weak. However, this interaction is enhanced by additional doping of carbon surfaces or their functionalization by oxygen-containing surface groups. Results of calculations are discussed in comparison with experimental data obtained from optical diffuse reflection, Raman scattering, FTIR absorption, and photoluminescence measurements performed for "nanocellulose"-graphene" nanocomposites.

Assumptions regarding possible relationship between doping and functionalization of carbon surface and the efficiency of adsorption of cellulose molecules by CNS are made.

ACKNOWLEDGMENTS

The calculations were performed using Bem supercomputer of Wroclaw Center for Networking and Supercomputing (grant no. 488).

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Lithium-Induced Reorientation of Few-Layer MoS_2 Films

Michaela Sojkova[1*], Igor Píš[2], Jana Hrdá[1], Tatiana Vojteková[1], Lenka Pribusová Slušná[1], Karol Végsö[3], Peter Šiffalovič[4], Peter Nádaždy[1], Edmund Dobročka[1], Miloš Krbal[5], Paul Fons[6], Frans Munnich[7], Elena Magnano[2], Martin Hulman[8, 9], Federica Bondino[2]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *IOM-CNR, Istituto Officina dei Materiali, S.S. 14 km – 163.5, 34149 Basovizza, Trieste, Italy (Italy)*

[3] *Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 84511 Bratislava (Slovakia)*

[4] *Centre of Excellence for Advanced Materials Application, Dúbravská cesta 9, 84511 Bratislava (Slovakia)*

[5] *Center of Materials and Nanotechnologies (CEMNAT), Faculty of Chemical Technology, University of Pardubice, Legions Square 565, 530 02 Pardubice, Czech Republic (Czech Republic)*

[6] *Faculty of Science and Technology, Keio University, Department of Electronics and Electrical Engineering, 223-8522 3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Kanagawa 223-8522, Japan (Japan)*

[7] *Helmholtz-Zentrum Dresden-Rossendorf, e.V. Bautzner Landstrasse 400, D-01328 Dresden, Germany (Germany)*

[8] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*

[9] *Danubia NanoTech s.r.o., Bratislava (Slovakia)*

*michaela.sojkova@savba.sk

Abstract ID #NSS-0684

Molybdenum disulfide (MoS_2) few-layer films have gained considerable attention for their possible applications in electronics, and optics, and also as a promising material for energy conversion and storage.[1,2] Intercalating alkali metals, like lithium, offers the opportunity to engineer the electronic properties of MoS_2.[3] However, the influence of lithium on the growth of MoS_2 layers has not been fully explored. Here, we have studied the influence of lithium on the structural and optical properties of MoS_2 few-layer films prepared using a new method based on one-zone sulfurization with Li_2S as a source of lithium. This method enables the incorporation of Li into octahedral and tetrahedral sites of the already prepared MoS_2 films or during the MoS_2 formation. The measurements show the long-term stability and preserved chemical composition of the horizontally aligned Li-doped MoS_2.

Our results discover an important effect of lithium promoting the epitaxial growth and horizontal alignment of the films. Moreover, we observed a vertical-to-horizontal reorientation in vertically aligned MoS_2 films upon lithiation. Since vertically and horizontally oriented films exhibit distinct electronic, chemical, and optical properties, control over the MoS_2 crystallographic orientation will be crucial in engineering next-generation devices incorporating MoS_2 layers.

ACKNOWLEDGMENTS

The research leading to this result has been supported by the project CALIPSOplus and NFFA-Europe under Grant Agreement 730872 and 654360 from the EU Framework Programme for Research and Innovation HORIZON 2020. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101007417 having benefited from the access provided by IOM-CNR in Trieste (Italy) within the framework of the NFFA-Europe Pilot Transnational Access Activity, proposal ID101. XPS and XANES measurements carried out at BACH beamline of CNR at Elettra synchrotron facility in Trieste were performed thanks to the mobility project CNR-SAV-20-03. This work was supported by the Slovak Research and Development Agency (Nos. APVV-21-0231, APVV-21-0278, and APVV-19-0365) and Slovak Grant Agency for Science (VEGA 2/0059/21).

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High Carrier Mobility $PtSe_2$ Thin Films Grown by One-Zone Selenization on Various Substrates

Jana Hrdá[1*], Tatiana Vojteková[1], Lenka Pribusová Slušná[1], Ondrej Pohorelec[2], Dagmar Gregušová[3], Martin Hulman[4, 5], Michaela Sojkova[1]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Institute of Electrical Engineering, Slovak Academy of Sciences (Slovakia)*

[3] *Institute of Electrical Engineering, Slovak Academy of Sciences. 841 04 Dubravska cesta 9, Bratislava (Slovakia)*

[4] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*

[5] *Danubia NanoTech s.r.o., Bratislava (Slovakia)*

*jana.hrda@savba.sk

Abstract ID #NSS-0685

Two-dimensional (2D) materials have attracted significant attention after the discovery of graphene. Recently, layered 2D transition metal dichalcogenides (TMDs) materials have been extensively studied due to their promising application in various fields, such as nanoelectronics, spintronics, and optoelectronics. Platinum diselenide ($PtSe_2$) belongs to the family of noble TMDs with tunable bandgap, high carrier mobility, and air stability, which makes it a suitable candidate for various applications. Here, we present the fabrication of large-area $PtSe_2$ thin films using one-zone selenization of magnetron sputtered Pt layers of various thicknesses. Like other growing parameters (temperature, heating ramp, nitrogen flow, etc.), the substrate influences the final alignment of $PtSe_2$ thin films and thus its properties, especially charge carrier mobility. In our work, we studied the influence of different substrates (c-plane sapphire, Si, Si/SiO_2, and annealed Si/SiO_2), and synthesis conditions on the structural and electrical properties of as-prepared $PtSe_2$ few-layer films. $PtSe_2$ films grown on c-plane sapphire substrates tend to be ordered in-plane, similar to the epitaxial growth. Moreover, those film exhibits high charge carrier mobility. Conversely, $PtSe_2$ films that are grown on non-crystalline substrates reveal low crystallinity and thus a reduction in carrier mobility. In the case of annealed Si/SiO_2 substrates, we are able to grow films comparable to those on the sapphire substrates. By decreasing the heating ramp, the film's grain size and consequently charge carrier mobility is increased.

ACKNOWLEDGMENTS

This work was supported by the Slovak Research and Development Agency (Nos. APVV-21-0231, APVV-21-0278, and APVV-19-0365) and Slovak Grant Agency for Science (VEGA 2/0059/21). This study was performed during the implementation of the project Building up Centre for advanced material application of the Slovak Academy of Sciences, ITMS project code 313021T081 supported by Research and Innovation Operational Programme funded by the ERDF. We acknowledge Dr. I. Píš and Dr. F. Bondino for the XPS measurements.

Electrical and Structural Properties of PEDOT:PSS Polymer Matrices Reinforced with Carbon Nanotubes

Illia Zhydenko[1*], Halyna Klym[1], Dmytro Chalyy[2], Ivan Karbovnyk[3]
[1] *Lviv Polytechnic National University (Ukraine)*
[2] *Lviv State University of Life Safety (Ukraine)*
[3] *Ivan Franko National University of Lviv (Ukraine)*
*i.zhydenko@i.ua

Abstract ID #NSS-0724

In the field of materials science, understanding the properties and behavior of polymers is of utmost importance in the development of new and improved materials for various applications. One area of research involves the use of carbon nanotubes (CNTs) as inclusions in polymer layers, which has shown promise in enhancing their electrical conductivity.

In a recent study, researchers experimentally analyzed the structural features and electrical behavior of PEDOT:PSS polymer layers with inclusions of high-purity single-walled (SWCNTs) or multi-walled carbon nanotubes (MWCNTs). Both types of nanotubes are known for their high structural perfection, making them ideal candidates for this type of research.

The results of the investigation showed that all samples exhibited the lowest impedance (highest conductivity) at room temperature, with conductivity decreasing upon cooling. The trend observed was that the real part of the impedance (Re(Z)) slightly increased with frequency from 1 kHz up to a certain threshold frequency, after which it dropped rapidly. This threshold frequency was found to be around 100 kHz for pure PEDOT:PSS and PEDOT:PSS/SWCNTs samples, and slightly lower for composite layers with MWCNTs.

The effect of temperature on the impedance of the polymer/CNT composite layers deserves special attention. The real part of the impedance (Re(Z)) was found to increase drastically at a certain temperature, which varied depending on the composition of the sample. For pure polymer samples, this increase occurred at temperatures as low as 80-90 K, with Re(Z) almost reaching the limit of measurability below 60 K. However, for layers reinforced with SWCNTs, the increase in impedance was more gradual, and even more so for MWCNTs-reinforced composites. In the latter case, reliable measurements could be performed at temperatures as low as 40K.

The conditions for residual water storage in samples with incorporated CNTs were found to be potentially different due to the structural changes introduced by the nanofiller. As a result, the time needed for complete water removal varied, with the process eventually finishing at different temperatures. This was further supported by the fact that samples with MWCNTs showed slower growth of real impedance with decreasing temperature and generally had higher conductivity at the lowest measured temperatures.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Education and Science of Ukraine (Project No 0122U000807).

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Bio-enabled Functional Nanomaterials: From Actuating Flexible Magnets to Photonically-Assisted Logic

Vladimir Tsukruk*
Georgia Institute of Technology (United States)
*vladimir@mse.gatech.edu

Abstract ID #NSS-0729

Bio-enabled hybrid nanomaterials represent a novel class of functional materials, which uses bio-derived materials, bioinspiration and biomimetic approaches to design functional nanomaterials and structures with co-assembled biological and synthetic components to bring best of two worlds: diverse adaptive photonic functions and mechanical strength, flexibility, and scalability [1]. In this talk, we summarize our recent results on functional hybrid nanomaterials from chiral nematic polysaccharides co-assembled with graphene oxides, magnetic nanoparticles, and quantum dots for adaptive chiroptical materials, magnetic photonic materials and photonic multi-value logic thin film electronics.

Firstly, we discuss robust photonic nanomaterials from cellulose nanocrystals and nanofibers decorated with highly photoluminescent organic dyes, quantum dots and quantum nanowires for tailored emission of linear and circular polarized light [2, 3]. Secondly, we present results on magnetically steerable uniform photonic organization of cellulose nanocrystals decorated with superparamagnetic nanoparticles [4]. Assembly under weak magnetic field gradients enables transformation from helicoidal cholesteric to uniaxial nematic phase with near-perfect orientation order parameter was achieved across large areas, enhanced mechanical robustness, and fast actuation ability. Finally, we demonstrate biophotonic field effect transistors with multi-valued logic elements for dramatically elevated encryption ability [5].

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Structural and Optical Properties of Nano-Phases in Ar^+ Sputtered SiC Surfaces

Divya Gupta*, Sanjeev Aggarwal
Kurukshetra University (India)

* divyagupta2017@kuk.ac.in

Abstract ID #NSS-0741

Silicon Carbide (SiC) is a fascinating wide band gap semiconductor with superior properties, such as excellent thermal conductivity, high breakdown field strength, and excellent physical and chemical stability. In this regard, present work investigates the structural behavior of as-deposited and argon sputtered SiC thin films at varying fluences keeping ion incidence at 50 degree. Raman spectroscopy and UV-Vis spectroscopy have been employed for assessing the structural transformations under present case. An increase in the optical absorption and a shifting of absorption edge towards longer wavelengths were observed. The observed structural behavior is attributed to the different degree of sputtering yield at different argon ion fluences and non-stochiometric sputtering of silicon and carbon.

Development of Defects in the Growth of Lead-Halide Perovskite Films

Nada Mrkyvkova[1], Vladimir Held[1], Karol Vegso[1], Peter Nadazdy[1], Martin Ledinsky[2], Matej Jergel[1], Frank Schreiber[3], Peter Siffalovic[4*]

[1] *Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 84511 Bratislava (Slovakia)*
[2] *FZÚ - Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6 (Czech Republic)*
[3] *Institute of Applied Physics, University of Tübingen, 72076 Tübingen, Germany (Germany)*
[4] *Institute of Physics, Slovak Academy of Sciences (Slovakia)*

* siffalov@gmail.com

Abstract ID #NSS-0751

Lead-halide perovskites are among the most intensively researched materials in photovoltaics and optoelectronics because of their high energy conversion efficiency and ease of fabrication at low temperatures. However, further performance enhancement necessitates a reduction in non-radiative defects and possible structural improvements. In this contribution, a unique combination of in-situ photoluminescence (PL) spectroscopy and grazing-incidence small/wide-angle X-ray scattering (GI-SAXS/WAXS) is employed to investigate the structural and optoelectronic kinetics of perovskite layer formation. We compare the growth of vapor-deposited and spin-coated perovskites. In the experiments, we track the format of perovskite from early nucleation and monitor the changes in structure and defect density in real time. In both cases, the growth of perovskite nanocrystals is followed by a rapid increase in PL intensity and a significant PL redshift. Moreover, the overall non-monotonic character of PL intensity during perovskite formation reflects the perovskite phase volume and defect states at the perovskite layer surface and grain boundaries. Most interestingly, the evolution of PL intensity is similar for both - wet-cast and vapor-based - perovskite fabrication techniques. This observation indicates the existence of an analogous mechanism of defect development, despite the fact that different chemical processes are involved during perovskite formation.

ACKNOWLEDGMENTS

This work was supported by APVV-21-0297, APVV-20-0111, SK-CZ-RD-21-0043, BMBF and DFG, and ITMS 313021T081.

Using Nanoparticles to Study the Axial Structure of a Gas Discharge

Valeriy Lisovskiy*, Stanislav Dudin, Sergiy Bogatyrenko, Pavlo Platonov
V.N. Karazin Kharkiv National University, Kharkiv (Ukraine)
* lisovskiy@yahoo.com

Abstract ID #NSS-0763

In this work, we study the processes of nanoparticle formation and deposition from acetylene plasma in the glow, RF capacitive, and pulsed discharges. The experiments were carried out in a discharge tube with an inner diameter of 56 mm and vertically arranged electrodes, the distance between which was 77.5 mm. Nanoparticles were collected on the glass slides and grids for subsequent analysis with a transmission electron microscope. Either a DC voltage, or a bipolar pulsed voltage (22-96 kHz, a duty cycle 15-65 %), or an RF voltage (13.56 MHz) was applied to the potential electrode while the second electrode was grounded. The experiments were carried out in the acetylene pressure range of 0.05–0.2 Torr.

With the help of simultaneous photo and video recordings of a burning discharge, as well as analysis of nanoparticles deposited on the slide, we managed to find out in which parts of the discharge the formation and retention of nanoparticles is possible. In order for a large number of nanoparticles with sizes of 10s to 100s of nanometers to fall on a certain section of the sample, it is necessary to create conditions in the plasma above this section of the sample for their growth with simultaneous retention. The ambipolar electric field does not allow small nanoparticles to escape toward the walls of the tube and the sample, but it does not prevent the axial escape of nanoparticles, for example, to the anode surface in a glow discharge. Therefore, nanoparticles are predominantly formed and retained, for example, in the region of the existence of a potential well on the axial profile of the electric field. In the glow discharge, the largest number of nanoparticles was deposited on the sample from the negative glow region of the discharge, in which a potential well for electrons and negatively charged nanoparticles appears. In the RF discharge with a narrow distance between the electrodes, nanoparticles are deposited on the sample from the entire region of the quasi-neutral plasma, since in this case the RF discharge has a symmetrical profile of the time-averaged plasma potential. However, when we used a distance between the electrodes of 77.5 mm, part of the RF current is closed as on the grounded electrode as also on the grounded parts of the devices surrounding the discharge tube. Therefore, the axial profile of the average plasma potential ceases to be symmetrical, and the nanoparticles are deposited preferentially in the region near the potential RF electrode.

Therefore, the study of the places of predominant deposition of nanoparticles from the plasma on the sample makes it possible to determine the presence of potential wells in the axial direction, which is difficult to do under the conditions of a polymer-forming plasma, for example, using other local measurements (e.g. Langmuir probes). Analysis of the diameter of deposited nanoparticles can also be used to estimate the internal parameters of the plasma in the region of their retention.

ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Ukraine in the framework of the project 2021.01/0204.

Surface Termination Dependent Topological States on InBi(001)

Maria Christine Richter[1*], Olivier Heckmann[1], Jan Minar[2], Jean-Michel Mariot[3], Johan Adell[4], Mats Leandersson[4], Janusz Sadowski[5], Jurgen Braun[6], Hubert Ebert[6], Jonathan Denlinger[7], Ivana Vobornik[8], Jun Fujii[9], Pavol Sutta[10], Gavin Bell[11], Martin Gmitra[12], Karol Hricovini[13]

[1] *LPMS CY Cergy Paris Université (France)*
[2] *New Technologies Research Centre, University of West Bohemia (Czech Republic)*
[3] *Laboratoire de Chimie Physique{Matiere et Rayonnement, Sorbonne Universite (France)*
[4] *MAX IV Laboratory, Lund University (Sweden)*
[5] *Institute of Physics, Polish Academy of Sciences (Poland)*
[6] *Department Chemie, Ludwig-Maximilians-Universitat Munchen (Germany)*
[7] *Advanced Light Source, Lawrence Berkeley National Laboratory (United States)*
[8] *TASC Laboratory, Istituto Ocina dei Materiali, CNR (Italy)*
[9] *TASC Laboratory, Istituto Ocina dei Materiali (Italy)*
[10] *Institute of Physics, Pavol Jozef Šafárik University in Košice (Slovakia)*
[11] *Warwick University (United Kingdom)*
[12] *Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)*
[13] *LPMS CY Cergy Paris Université and LIDYL, Universite Paris-Saclay, CEA (France)*
*Christine.Richter@cyu.fr

Abstract ID #NSS-0765

InBi is a non-symmorphic semimetal, lacking a mirror plane along the [001] axis, which exhibits a 1D nodal line in the vicinity of the X point. Here we show how InBi(001) can be formed on a III-V semiconductor substrate by depositing Bi on to a In-rich InAs(111)A. ARPES measurements reveal new topological electronic surface states, close to the M hight symmetry point. Theoretical calculations based on relativistic density functional theory with a one step-model photoemission model clarify the relationship between InBi(001) surface termination and these surface states, supporting a predominant Bi bilayer termination. A tight-binding model based on the Bi bilayer with only Bi-Bi hopping terms, and no Bi-In interaction, reproduces the calculated spin texture. Our study gives a consistent physical picture of the topological surface electronic structure of InBi(001) based on an intact Bi bilayer rather than a surface formed by splitting to a Bi monolayer termination.

Effect of Nanoconfining PLGA Shell on the Self-Assembly of Indigo Carmine

Shaked Ashkenazi, Iris Weitz*
Braude College of Engineering Karmiel (Israel)
* irisweitz@braude.ac.il

Abstract ID #NSS-0767

Molecular self-assembly, particularly under 3D spherical confinement, is driven by inherent properties of molecules, as well as the confining system, both play a dominant role in the final self-assembled structure [1, 2]. We recently proposed a novel approach for confinement, in which the core of polymeric nanocapsules was used to entrap organic dye molecules (e.g., indigo carmine), that subsequently organize into rolled up lamellar molecular sheets forming scroll structures [3]. To examine the effect of the confining shell composed by polymeric encapsulating materials, the high molecular weight poly-lactide (PLA) was replaced with low molecular weight poly (lactide-co-glycolide) (PLGA). The PLGA based confining system was prepared by water-in-oil-in-water ($W_1/O/W_2$) double emulsions. Various techniques were used to analyze the physicochemical properties of the self-assembled dye loaded nanocapsules, in terms of particle morphology, size distribution, surface charge, core content, shell composition, loading capacity, and thermal stability. These techniques also served to evaluate the interactions of the dye and its lamellar nanosheets with the interior wall of the capsule shell. The results show, given the same molecular building unit for self-assembling, that the confining shell charge predominates the spatial growth and the direction of assembled organic dye molecules. This provides a further understanding of the polymeric nanocapsule cavities as an emerging viable platform for practical self-assembling applications.

ACKNOWLEDGMENTS

The research was supported by Braude College of Engineering Karmiel.

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Magnetic Nanowires as Growth Catalysts for Carbon Nanotubes

Roman Kolisnyk[1*], Bethanie Stadler[1], Morgen Smith[2], Placidus Amama[2], Jeanne Riga[3]
[1] *University of Minnesota Twin Cities (United States)*
[2] *Kansas State University (United States)*
[3] *Air Force Research Laboratory (United States)*
* rkolisny@umn.edu

Abstract ID #NSS-0769

Remarkable intrinsic properties of carbon nanotubes (CNTs) make them potential candidates for nanoscale applications. Selection of a suitable substrate material is very important to enhance the properties of CNT-based devices. The form of the substrate/catalyst also contributes to the CNT properties. Metallic nanowires are not commonly used as catalysts, but since they are nanoscale, it may be easier to nucleate nanoparticles on their surface before growing the CNTs. Such studies have already been reported for possible application of metal nanowire heterostructures as multi-structures with CNTs [1-2]. However, there are no works reported so far in which the influence of nanowire length and diameter as catalysts for CNT growth and properties was studied. Here, we show the ability to grow CNTs atop nickel nanowires with different aspect ratio inside 50μm-thick anodic alumina oxide templates. The diameters were varied by electrochemical deposition of Ni into various sized nanopores, and the distance from the top of the Ni nanowires to the top of the AAO template was varied by depositing full- and half-length Ni. We found that it is possible to control the CNTs density. For example, 200nm nanowires with full lengths (> 45μm) produce a forest-like structure on the template surface, while smaller diameter, half-length nanowires led to a reduction of CNT density. This difference in density is likely associated with difficulties of gas diffusion inside the pores and reaction with catalyst. Also, higher diameters act as nucleation sites for several CNTs at the same location. These multistage structures, due to their synergetic properties, can find applications in sensors or capacitors, while the present work focused on constructing efficient field emission cathodes.

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Morphology and Optical Properties of Porous Silicon Filled with Luminescent Oxide Dielectric Nanoparticles

Alla Kuryliuk[1*], Volodymyr Boyko[2], Olga Gomenyuk[3], Serhii Nedilko[1, 4], Kateryna Terebilenko[1], Petro Teselko[1], Vasyl Scherbatskyi[1], Vadym Sheludko[3], Viktoria Shevchenko[1], Vitalii Chornii[2,1]

[1] *Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *National University of Life and Environmental Sciences of Ukraine (Ukraine)*
[3] *Oleksandr Dovzhenko Hlukhiv National Pedagogical University (Ukraine)*
[4] *Institute of Physics Polish Academy of Sciences (Poland)*

*kurylyuk_a2008@ukr.net

Abstract ID #NSS-0771

A wide range of possible applications of multifunctional composites based on porous silicon (PSi) is determined by its attractive characteristics, e.g., high specific surface, pores volume, and size of the pores. The simple way of PSi surface chemistry modifying and the easy procedure of the PSi films fabrication are also advantages for the sensors based on PSi. A high reactivity of surface makes the physicochemical properties of PSi very sensitive to its environment. So, the changes in the chemical, electrical, and optical properties of the PSi can be used to develop chemical, biological, and optical sensors [1].

Mainly, the sensing principle of an optical sensor is based on the changing of PSi photonic structure effective refractive index. The features of porous silicon own photoluminescence (PL) can also be used for the development of optical sensors. However, characteristics of the PSi own PL are very sensitive to various factors, that complicates the analysis of the PL data measured. Therefore, the use of an additional material (filler) with predictable luminescent characteristics is a way to improve the efficiency of luminescent sensors based on PSi.

Bismuth phosphate doped with praseodymium ($BiPO_4$:Pr), and potassium europium phosphate tungstate ($K_2Eu(PO_4)(WO_4)$) were used as oxide fillers in this work. The details of the synthesis procedures of these oxides can be found here [2,3]. PSi matrices were formed by anodizing of p^+ type (100) silicon wafers with a resistivity of 0.01 - 0.02 Ω cm. The average diameter of the pores varied in the range 10 - 30 nm. Pores filling was carried out by soaking the porous silicon plates in the aqueous suspension of the noted above oxides.

The samples of the PSi nanocomposites were characterized with use of the powder X-Ray diffraction, scanning electron and optical microscopy, energy dispersive X-Ray analysis, FTIR, optical absorption and the PL spectroscopy.

A comparative analysis of the data obtained for the samples of starting silicon, starting PSi, both of starting silicon and porous silicon covered with the luminescent oxide layers was performed.

The PL data showed changes in the spectral characteristics of the composites in comparison with their starting constituents. E.g, the starting PSi, even when excited by powerful laser radiation, shows low-intensity PL, which is described by a wide multicomponent band in the range of 490 - 800 nm. The PL spectra of the PSi nanocomposites mainly correspond to the typical emission of the RE^{3+} ions caused by f-f radiation transitions. At the same time, some spectral details unusual for the f-f luminescence of the "free" oxide powders were observed in the spectra of the composites.

The relation between spectral characteristics of PL, IR absorption, light reflection etc., and conditions of the samples preparation and treatment were discussed considering the interactions between the components of the PSi nanocomposites.

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Dewetting-Assisted Patterning: A Lithography-Free Route to Synthesize Black and Colored Silicon

Amin Farhadi*, Gilles R. Bourret
Department of Chemistry and Physics of Materials, University of Salzburg (Austria)
*amin.farhadi@plus.ac.at

Abstract ID #NSS-0779

Thanks to its high abundancy, optimum band-gap for solar absorption and tunable optoelectronic properties, silicon has become the semiconductor of choice for many applications, ranging from microelectronics to photovoltaics. Micro-, and nanostructuring silicon into vertically-oriented wires can enhance further Si's optoelectronic properties, which is particularly relevant for photo(electro-)catalytic and sensing applications [1]. Here we report the use of thermal dewetting to structure gold-based catalytic etching masks for metal-assisted chemical etching (MACE). The approach involves the low-temperature dewetting of metal films to generate holey meshes with tunable morphology and dimension. Combined with MACE, thermal dewetting can be used to synthesize microporous Si, Si nanotubes, Si nanowires and Si nanowalls with defined dimensions. Patterning via dewetting provides a simple, bench-top route, to prepare black and colored silicon. We report the lithography-free fabrication of silicon nanowires with sub-100 nm lateral dimensions that sustain leaky wave-guiding modes, giving rise to vibrant colors. To-date, the fabrication of colored silicon has relied on complicated nanoscale patterning processes. Patterning via dewetting provides a simpler alternative that eliminates this requirement [2].

ACKNOWLEDGMENTS

A.F. gratefully acknowledges support from the Austrian Academy of Science (ÖAW) for a full doctoral scholarship (DOC stipendium scheme).

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Study of Defects in the ZnO/SiC/Porous-Si/Si Heterostructure

Valeriy Kidalov[1], O. Y. Gudimenko[2], Yuriy Bacherikov[3], V.A. Baturin[4], Olga Okhrimenko[3], O. Yu. Karpenko[4], Sergei Simchenko[5,6*]

[1] *Dmytro Motornyi Tavria State Agrotechnological University (Ukraine)*
[2] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine (Ukraine)*
[3] *V. Lashkaryov Institute of Semicon-ductor Physics National Academy of Sciences of Ukraine (Ukraine)*
[4] *Institute of Applied Physics, National Academy of Sciences of Ukraine (Ukraine)*
[5] *State University of Telecommunications (Ukraine)*
[6] *Department of Higher Mathematics, Mathematical Modeling and Physics State University Telecommunications (Ukraine)*

* sstehnology85@gmail.com

Abstract ID #NSS-0784

This research presents the results of obtaining and studying the ZnO/SiC/porous-Si/Si heterostructure. Obtaining the ZnO/SiC/porous-Si/Si heterostructure was made in several stages: electrochemical etching of single-crystal Si plates (100); deposition of SiC films by the method of solid-phase epitaxy; deposition of ZnO films by magnetron sputtering. The samples were divided into two groups depending on the conditions of the deposition process of ZnO films, namely, for the first batch of samples, the oxygen pressure of PO2 was 0.06 Pa, for the second - 0.1 Pa. The thickness of ZnO films is ~290 nm and ~970 nm for the first and second groups, respectively. According to the X-ray diffraction pattern of ZnO films grown at 0.1 Pa, there is a band with a maximum of 34.37°, the full width at half maximum of this band is 0.731°. For the sample obtained at the pressure of 0.06 Pa, there is a band with a maximum of 34.40°, the full width at half maximum of this peak is 0.582°. The presence of a triplet in the range of 31-36 degrees, for this sample, indicates the presence of a polycrystalline hexagonal phase of ZnO. The residual stress takes negative values, which is an indication of compressive biaxial stress. The low value of the residual stress (0.511 and 0.287 GPa) indicates the high quality of the obtained ZnO films.

Synthesis and Thermal Decomposition of Magnesium Whitlockite

Ligita Valeikiene[1*], Jonas Stadulis[1], Vytautas Klimavičius[2], Tomoyo Goto[3], Tohru Sekino[3], Aleksej Zarkov[4]

[1] *Vilnius University (Lithuania)*
[2] *Institute of Chemical Physics, Vilnius University, Sauletekio 3, LT-10257, Vilnius, Lithuania (Lithuania)*
[3] *Osaka University (Japan)*
[4] *Institute of Chemistry, Vilnius University, Naugarduko g. 24, LT-03225, Vilnius, Lithuania (Lithuania)*
* ligita.valeikiene@chgf.vu.lt

Abstract ID #NSS-0789

Magnesium whitlockite (Mg-WH, $Ca_{18}Mg_2(HPO_4)_2(PO_4)_{12}$) is a promising candidate for biomedical application in bone regeneration; however, the fabrication of Mg-WH bioceramics by conventional methods is limited by its thermal stability. Mg-WH is known to be thermally unstable and decomposes upon heating. The mechanism of thermal decomposition and phase evolution was not comprehensively investigated so far.

In the present work, Mg-WH was synthesized by dissolution-precipitation process under hydrothermal conditions. Thermally induced degradation of the synthesized powders was investigated in detail by combining X-ray diffraction analysis (XRD), infrared spectroscopy (FTIR), Raman spectroscopy as well as 1H and 31P solid-state nuclear magnetic resonance (NMR). As-prepared Mg-WH powders were annealed at different temperatures in the range from 400 °C to 1300 °C with a step of 100 °C. It was determined that thermal decomposition starts at around 700 °C with the formation of beta-tricalcium phosphate (β-TCP, $Ca_3(PO_4)_2$) and a mixture of two $Ca_2P_2O_7$ polymorphs. Thermal decomposition occurs gradually and co-existence of both Mg-WH and β-TCP phases was observed in a broad temperature range up to 1200 °C. Complete disappearance of HPO_4^{2-} structural unit was confirmed only after annealing at 1300 °C following by melting at 1400 °C.

ACKNOWLEDGMENTS

This research was funded by a grant WHITCERAM (No. S-LJB-22-1) from the Research Council of Lithuania.

Core@Shell@Shell Nano-Photo Reactors Development Using Al:$SrTiO_3$@FeOOH@SiO_2 System for Photocatalytic Water Splitting

Ioana Radu[1], Tiberiu Roman[1, 2, 3*], Adrian Iulian Borhan[1], Georgiana Andreea Bulai[2], Daniel Gherca[3], Aurel Pui[1]

[1] *"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, Carol I nr. 11 Blvd., Iasi 700506, Romania (Romania)*

[2] *Integrated Center of Environmental Science Studies in the North-Eastern Development Region (CERNESIM), Department of Exact and Natural Sciences, Institute of Interdisciplinary Research, Alexandru Ioan Cuza University of Iasi, 700506 Iasi, Romania (Romania)*

[3] *National Institute of Research and Development for Technical Physics, 47 Mangeron Boulevard, Iasi 700050, Romania (Romania)*

* tiberiu.roman@chem.uaic.ro

Abstract ID #NSS-0792

Self-assembled materials development aiming for the reduction in the environmental pollution and high-efficiency green energy is focused to fulfill the zero-emission international policies. Inorganic materials had attracted a lot of attention lately for electronic and energy production-related applications [1,2]. The perovskite type of materials such as $SrTiO_3$ (STO) possess a good photocatalytic activity under UV-light, but it is verry much restricted in the VIS-domain due to its wide band gap [3]. One of the most convenient is doping the STO with a compatible enhancing element such as Al [4] or even to design a multi-layered material capable of VIS activity. Thus, we managed to synthesize a material core@shell@shell type coning of Al:SrTiO3@FeOOH@SiO_2 in three stages and enhances its photo-catalytical activity by progressively lowering its bang gap (E-g) from 3.34 eV specific for Al:STO to 1.94 eV for Al:$SrTiO_3$@FeOOH@SiO_2 system. Visible morphological and dimensional aspects are noticed during the layering process. Also, the PXRD suggests the presence of each crystallographic phase in the final material starting with the core ($SrTiO_3$ – Al doped), first layer (FeOOH – the δ phase) and the second layer consisting of SiO_2- phase. We consider that the designed material will be of interest in the photocatalytic activity and water splitting applications as the band gap is lowered each step of the process. Also, the meta-stable form of FeOOH could lead to a new type of materials consisting of core@shell@void@shell as under temperature exposure the FeOOH is transformed in a denser Fe_2O_3 type of shell. The photocatalytic water splitting activities were carried out under the visible light irradiation at room temperature and evolved gases being in-situ real-time quantified using H_2/O_2 microsensors.

ACKNOWLEDGMENTS

This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS-UEFISCDI, project number PN-III-P4-ID-PCE-2020-1385, within PNCDI III.

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Chemical Vapor Deposition Growth of Monolayer and Few-Layer $MoSe_2$

Magdalena Precnerova[1,2*], Marián Precner[3], Peter Hutár[2], Viera Skákalová[2], Ján Šoltýs[2]
[1] *Centre For Advanced Materials Application CEMEA, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava (Slovakia)*
[2] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava (Slovakia)*
[3] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*
*michaela.sojkova@savba.sk
Abstract ID #NSS-0800

Transition metal dichalcogenides (TMDs) include a huge class of two-dimensional layered materials with unique chemical and physical properties. [1] Within the TMD family, molybdenum diselenide ($MoSe_2$) has properties dependent upon the number of layers.

With a decrease of $MoSe_2$ layers from multiple layers to a few layers or even a single layer, there is a change in its electron band gap from the original indirect to the direct band gap.

These tuneable properties of $MoSe_2$ make it an appealing material for electrical and optical applications such as field effect transistors (FETs), photovoltaic cells, light emitting diodes (LEDs), and photodetectors. [2] However, the synthesis of high-quality monolayer $MoSe_2$ with large grain size and good uniformity still remains a significant challenge. [3]

In this work, mono- and few-layers of $MoSe_2$ were synthesized using MoO_3 and Se powder as precursors on Si/SiO_2, sapphire, and Si/SiO_2/graphene substrates. The thin layers were grown via a controllable chemical vapor deposition (CVD) method at atmospheric pressure, which led to the formation of large-size crystals with a typical triangular shape and highly uniform continuous films with a clean surface.

By changing the relevant growth parameters, the thickness of the films was able to tune from few- to mono-layer which was confirmed by Raman spectroscopy and photoluminescence measurement. In addition, the stoichiometric composition of prepared $MoSe_2$ layers was 1:2 confirmed by energy dispersive spectroscopy.

The results of our work spread the research in the synthesis of uniform $MoSe_2$ monolayer and the influence of growth parameters on chemical vapor deposition which can be useful for the synthesis of other 2D materials.

ACKNOWLEDGMENTS

This work was supported by Slovak Grant Agency VEGA (Project No. 2/0168/22).

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Geometrically Well-Defined Nanostructure Arrays Replicated from Designable Anodic Aluminum Oxide Templates for Optoelectronic Application

Rui Xu*, Denys Makarov
Helmholtz-Zentrum Dresden-Rossendorf e.V. (Germany)
* r.xu@hzdr.de

Abstract ID #NSS-0801

Advanced devices play a critical role for sustaining the ever-growing demands of our society for energy, information, health care, etc. To achieve high performance, devices with nanoscaled features are attracting more and more attentions by virtue of their unique and promising effects emerging at nanoscale [1]. Structural design and engineering of materials provides a versatile platform to optimize the device performance and improve the commercial competitivity. Regarding the structural engineering, controlling the geometrical parameters (i.e., size, shape, hetero-architecture, and spatial arrangement) of nanostructures have been the central aspects of investigations and practical applications. Low-cost high-yield template-guided techniques have been a workhorse for nanostructure fabrication. Here we report designable anodic aluminum oxide templates with well-defined pore features within templates in terms of in-plane and out-of-plane shape, size, spatial configuration, and pore combination [2, 3]. By using designable anodic aluminum oxide template, we realize well-defined controlling of nanostructures over the size, in-plane/out-of-plane shape, spatial arrangement, and hetero-architecture. Integrating well-defined nanostructures into optoelectronic devices (e.g., photoelectrochemical water splitting [4], solar steam generator [5], surface enhanced Raman spectroscopy [2]), the performance of nanodevices can be obviously enhanced due to the optical manipulation enabled by nanostructure supported surface plamson resonance effect.

ACKNOWLEDGMENTS

The authors thank Prof. Yong Lei, Dr. Liaoyong Wen, Dr. Yan Mi.

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Optical and Transport Properties of Polycrystalline Thin Layers of 2D-TMDC Semimetals

Martin Hulman[1,2*], Michaela Sojkova[3], Marián Precner[1], Lenka Pribusová Slušná[3], Tatiana Vojteková[3], Jana Hrdá[3], Jozef Kačmarčík[4], Martin Mosko[5], Edmund Dobročka[3]
[1] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*
[2] *Danubia NanoTech s.r.o., Bratislava (Slovakia)*
[3] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*
[4] *Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)*
[5] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*
* martin.hulman@savba.sk

Abstract ID #NSS-0803

Topological materials (TMs) are a new material category that has appeared in condensed matter physics. Weyl and Dirac topological semimetals (WSM, DSM) possess nontrivial band structures. In a DSM, a Dirac cone is formed at the cross point of bands with linear dispersion in the Brillouin zone. Either broken time-reversal or spatial inversion symmetry splits the Dirac cone into two Weyl cones. Some 2D materials from the family of transition metal dichalcogenides can host DSM or WSM states. Weyl fermions were proposed in 1T′ -WTe_2 and Td-$MoTe_2$, and 1T-$PtSe_2$ is considered a Dirac semimetal.

In the talk, I will first briefly introduce the way how we prepare thin layers of $MoTe_2$, WTe_2 and $PtSe_2$. A common feature of all samples is that the layers are polycrystalline with a thickness ranging from 2 nm to 30 nm. We will present the results of electric transport measurements at low temperatures and high magnetic fields performed on these layers. We observed indications of strong electron coupling, quantum interference and disorder-induced effects in some compounds. Transport measurements are supplemented by optical measurements performed mainly in the mid- and far-infrared regions. The optical conductivity extracted from these measurements carries information about the electronic structure near the Fermi level. We will also discuss how our experimental results and theoretical predictions agree for these compounds.

ACKNOWLEDGMENTS

Support from the APVV projects 19-0365, SK-AT-20-0020 is acknowledged.

Interactions of MXenes with Electromagnetic Waves – from Optoelectronic to Communication Technologies

Yury Gogotsi*
A.J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, 19104 (United States)

* gogotsi@drexel.edu

Abstract ID #NSS-0818

MXenes (carbides and nitrides of early transition metals) are a very large family of 2D materials. They have a chemical formula of $M_{n+1}X_nT_x$, where M represents a transition metal (Ti, Mo, Nb, V, Cr, etc.), X is either carbon and/or nitrogen (n = 1, 2, 3 or 4), and Tx represents surface terminations. The diversity in compositions (>50 MXenes have already been reported, >100 stoichiometric structures predicted), availability of solid solutions on M and X sites, and control of surface terminations, such as O, OH, F, Cl, S, etc., offer a plethora of structures and chemistries to investigate [1]. Combining the plasmonic properties with ease in processing, high electronic conductivity (over 20.000 S/cm) and mechanical properties, which exceed other solution-processable 2D materials, MXenes have the characteristics necessary to develop as optical and electronic materials [2]. Inherent to their 2D structure, the charge carriers responsible for MXene's optical responses and electronic transport are very close to an external interface that has exceptional ability to undergo reversible chemical and electrochemical reactions to add or change surface terminations. By design of the MXene composition, the carrier plasma can be rendered either sensitive to or uncommonly robust against the resulting changes in band structure and state-filling. MXenes offer chemically controlled optical and electronic properties that facilitate new ways of influencing material interactions with electromagnetic waves over visible light, IR, THz and even GHz ranges. Many technological advances can be enabled by these chemically responsive, conductive materials. MXenes have already shown great promise in applications such as electromagnetic interference shielding, antennas, electrodes and current collectors in energy storage devices. In this talk, I show that optical, electronic and transport properties of MXenes can be manipulated by tuning their chemical composition [3]. This presentation will also demonstrate electrochemical modulation of the optoelectronic properties and describe potential applications of MXenes as well as spectroscopic information, which can be applied to designing photonic and optoelectronic devices, such as electron transport layers for solar cells, optical sensors, electrochromic devices, metamaterials, EMI shields, etc. [1, 3].

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Morphological, Structural, Substructural Characteristics and Chemical Composition of $Zn2SnO_4$ Nanoparticles

Serhij Lyfar, Maksym Yermakov*, Roman Pshenychnyi, Olga Berezhna, Anatoliy Opanasyuk
Sumy State University (Ukraine)

*m.yermakov@ekt.sumdu.edu.ua

Abstract ID #NSS-0826

The work synthesized zinc stannate nanoparticles using KOH solution as a mineralizer by the hydrothermal method. The synthesis time ts was varied from 16 to 32 hours with an interval of 4 hours. Morphological, structural (lattice period, unit cell size), and substructural (size of coherent scattering regions, level of microdeformations, dislocation density) characteristics of nanoparticles and their chemical composition were studied. It was established that the particles obtained at ts = 16 h contained a mixture of phases, while the other samples were single-phase with a cubic structure of inverse spinel Zn_2SnO_4. As a result of the research, the temperature and time of synthesis of Zn_2SnO_4 nanoparticles were optimized.

ACKNOWLEDGMENTS

The research was performed under the financial support of the Ministry of Education and Science of Ukraine (0122U000787). This work was also supported by the National Research Foundation of Ukraine (project registration number: 2020.02 / 0313).

Simple Chemical Approach to 2D Metal Iodides/Graphene Heterostructures and their Properties

Viera Skákalová[1,2,3*], Kimmo Mustonen[3], Peter Kotrusz[2,1], Christoph Hofer[3], Thuy An Bui[3], Peter Hutár[4,5], Marián Precner[1]

[1] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*
[2] *Danubia NanoTech s.r.o., Bratislava (Slovakia)*
[3] *Faculty of Physics, University of Vienna, Vienna (Austria)*
[4] *Institute of Electrical Engineering SAS, Bratislava (Slovakia)*
[5] *Laboratory for Advanced Materials, Faculty of Natural Sciences, Comenius University, Ilkovičova 8, 84104 Bratislava (Slovakia)*

*viera.skakalova@savba.sk

Abstract ID #NSS-0829

The inertness and impermeability of its atomic structure makes graphene a suitable envelop to stabilizing less obvious two-dimensional (2D) structures. We invented a synthesis of 2D metal iodides, some of them inexistent at ambient conditions, embedded in graphene.

The 2D materials are grown by wet-chemical process at ambient conditions, directly within the space between two graphene oxide layers, while reducing the oxide groups in the same reaction step. This way, the newly formed 2D materials stay tightly encapsulated in graphene. Besides copper iodide, 2D-CuI, a material that normally only occurs in at elevated temperatures [1], a number of 2D structure like AgI, AuI_3, NiI_2, BiI_3 and EuI_2 have also been demonstrated. These 2D metal iodides are predicted to differ by their optical, magnetic and electrical properties relevant for novel quantum technologies.

Here, TEM images of the atomic structure of these 2D metal iodides complemented by EELS and XAS spectroscopies and additional characterization methods will be presented.

ACKNOWLEDGMENTS

Collaborators: Karol Hricovini and Christine Richter, CY Cergy-Paris University

Funding: Austrian Science Fund (FWF, project no. P35912), CEMEA of the Slovak Academy of Sciences (ITMS code 313021T081 of the Research & Innovation Programme), Joint Research Program V4-Japan (BGapEng)

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FT-IR Spectroscopy of $MoTe_2$ Thin Films

Tatiana Vojteková[1*], Lenka Pribusová Slušná[1], Jana Hrdá[1], Michaela Sojkova[1], Martin Hulman[2,3]
[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*
[2] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*
[3] *Danubia NanoTech s.r.o., Bratislava (Slovakia)*
* tatiana.vojtekova@gmail.com

Abstract ID #NSS-0830

Transition metal dichalcogenides (TMDs) have recently attracted great interest in condensed matter physics and materials science. They are well known due to their distinctive properties in photonics and optoelectronics. Molybdenum ditelluride ($MoTe_2$) belongs to this group of TMDs materials. $MoTe_2$ crystalises in three crystal symmetries: hexagonal (2H) $MoTe_2$ phase, monoclinic (1T) $MoTe_2$ and orthorhombic (Td) $MoTe_2$ phase. Changes in crystal structure and thickness cause changes in electronic structure from semiconducting to metallic. Under ambient conditions, $MoTe_2$ is thermodynamically stable in hexagonal structure and is an indirect bandgap semiconductor. When thinned to the monolayer, a transition occurs to a direct bandgap of 1.2 eV, close to Si and smaller than other TMDCs such as MoS_2 and WSe_2 [1]. Hexagonal $MoTe_2$ can be utilised as the channel material of field-effect transistors (FETs), while monoclinic $MoTe_2$ is expected to be a source material to realise a quantum spin Hall-effect device [2]. For the understanding of $MoTe_2$ materials applications, an understanding of the fundamental optical properties is required. The optical properties of the material are defined with optical constants such as refractive indices, dielectric function, or optical conductivity [3,4].

$MoTe_2$ thin films are uniform and large-area samples prepared by the CVD method at IEE SAS. Magnetron sputtered Mo film was annealed in CVD three-zone chamber with Te powder at a temperature of 680°C. For monoclinic structure, pre-oxidation of Mo film to form MoO_3 was necessary. The films coat the whole surface of the sapphire substrates with the size of 1x1 cm2. We distinguish the hexagonal and monoclinic structures with Raman spectroscopy, and the thickness of $MoTe_2$ layers was determined by measuring X-ray reflectivity (XRR). Optical measurements were performed in far- and near-infrared regions using the FTIR spectrometer Vertex 80v. Using transmission and reflection measurements and considering the substrate to be semi-infinite, we define the real and imaginary part of the refractive index for thin films of hexagonal and monoclinic $MoTe_2$ in the far and mid-infrared region. We observed changes in optical conductivity in connection with changes in the electronic structure of semiconducting hexagonal and semimetallic monoclinic $MoTe_2$.

ACKNOWLEDGMENTS

Authors acknowledge support from projects APVV-19-0365, APVV SK-AT-20-0020, SAS-MOST/JRP/2022/482/MSC and VEGA project 2/0046/23.

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MWCNTs Arrays Application to Reduce Interlayers Voids in a FRPC Produced by OoA Curing

Aleksei Shiverskii*, Sergey Abaimov
Center for Petroleum Science and Technology, Skolkovo Institute of Science and Technology (Russian Federation)
*aleksei.shiverskii@skoltech.ru

Abstract ID #NSS-0846

Nanosized materials become an integral part of solving many scientific and applied problems. Their using in composite polymeric materials gives the latter additional functionality [1]. The most popular technique to produce high-quality Fiber Reinforced Polymer Composites (FRPC) with low interlayers voids volume is autoclave curing. The low voids volume is important for critical applications, such as aerospace industry.

However, the industry wants to shift away from this expensive and energy-intensive technique towards more eco-friendly fabrication methods. The alternative techniques to obtain high quality FRPC are Out of Autoclave (OoA) curing, in particular curing by Vacuum Bag Only (VBO).

Here we show how embedding self-assembled vertically oriented arrays of Multi-Walled Carbon Nanotubes (MWCNTs) in interlayer region influences voids volume inside FRPC produced by OoA curing. To solve this task, we developed original equipment to grow arrays of vertical oriented MWCNTs with high surface density at atmospheric pressure. We found optimal geometrical parameters of MWCNTs allowing to reduce interlaminar voids volume into FRPC produced by VBO. The energy consumption and cost of our approach were in several times lower that at autoclave and oven curing. Our results show perspectives of OoA curing techniques for high quality FRPC production.

As the century of autoclave technology passes, the use of nanoadditives allows achieving similar results at a lower cost. Additionally, the network of MWCNTs inside FRPC opens a huge possibility for other applications, such as internal heaters to solve anti/de- icing problems [2], sensing applications, real time destruction monitoring systems [3], etc.

ACKNOWLEDGMENTS

This work was supported by the Skoltech NGP Program, the project "Multifunctional Fusion: Life-cycle enhancements via data-driven nanoengineering of advanced composite structures".

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New Approaches for New Materials: Exotic 2D Crystals from Table-Top Chemistry

Kimmo Mustonen[1*], Christoph Hofer[1], Peter Kotrusz[2,3], Alexander Markevich[1], Martin Hulman[3,2], Clemens Mangler[1], Toma Susi[1], Timothy J. Pennycook[4], Jannik C. Meyer[5,6,1], Jani Kotakoski[1], Viera Skákalová[3,2,1]

[1] *Faculty of Physics, University of Vienna, Vienna (Austria)*
[2] *Danubia NanoTech s.r.o., Bratislava (Slovakia)*
[3] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*
[4] *University of Antwerp EMAT, Antwerp (Belgium)*
[5] *Institute of Applied Physics, Eberhard Karls University of Tuebingen, Auf der Morgenstelle 10, D-72076, Tuebingen (Germany)*
[6] *Natural and Medical Sciences Institute at the University of Tuebingen, Markwiesenstr. 55, D-72770 Reutlingen (Germany)*

* kimmo.mustonen@univie.ac.at

Abstract ID #NSS-0875

A large number of bulk compounds have van der Waals phases at pressures and temperatures other than those of the ambient [1]. In principle, under the right physical conditions, similar to graphene and boron nitride, among others, they could be exfoliated down to thickness of a monolayer. In real world, however, the separation of single layers under for instance a temperature much higher than ambient, is virtually impossible, and beyond the crystallographic identification with X-ray or neutron diffraction experiments within high pressure anvils, the properties of such exotic phases remain largely unexplored. In my talk I will shortly outline an alternative route based on room temperature intercalation chemistry of graphene oxide that allows us to to access these exotic phases, and along with demonstrating the existence of 2D CuI [2] that normally exists only at high temperatures in ambient conditions, I will show also other exotic structures obtained by the same approach on the 2D limit.

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TRACK 2

“ELECTROCHEMISTRY OF NANOMATERIALS”

Iodine-doped Graphene as High Performance Electrocatalyst for Oxigen Reduction Reaction for PEM Fuel Cells

Adriana Marinoiu *

Institutefor Cryogenics and Isotopic Technologies – ICSI, Ramnicu Valcea, Romania (Romania)

* adriana.marinoiu@icsi.ro

Abstract ID #EN-0521

Graphene base materials have received attention as a substrate or a nanocomposite with nonmetallic particles for various applications. Besides the obvious desire for developing of catalysts more active than Pt, the theoretical understanding of the oxygen reduction reaction (ORR) mechanisms improved substantial in the last years, revealing that the key parameter for catalytic activity is the binding strength of oxygen to the catalyst surface. The halogen content in graphene dictates electronic, electrocatalytical and chemical proprieties of the resulting materials. It is due to the effect of the different electronegativity of halogen atoms, having a different ability of electron loss compared to O2−. The emerging application of iodine-doped (I-doped) graphene in PEM FC has been recently investigated as the novel nanomaterial for ORR. The significant interest caused by I-doped graphene is a result of its enhanced conductivity and improved catalytic activity for oxygen reduction reaction.Very inspiring cell performance was observed with I-doped graphene catalyst upon integration into cathode electrode. An aggressive accelerated test showed an insignificant degradation regarding ECSA, OCV and LSV but a gradually degradation regarding I-V performances.

ACKNOWLEDGMENTS

This work was carried out through the Nucleus Program, financed by the Ministry of Education and Research, Romania, project no. PN 23 15 01 03 and project number PN-III-P2-2.1-PED2021-0840 PED 695/2022.

Effect of N^+ Ion Implantation on Structural, Optical Properties and Dielectric Behavior of ZnO Thin-Films

Manjeet Mor *, Manish Kumar Vishwakarma, Puneet Jain

Indian Institute of Technology Roorkee (India)

* manjeet@ph.iitr.ac.in

Abstract ID #EN-0540

Zinc Oxide (ZnO) has wide range of applications in optoelectronics, gas sensors, and solar cells due to its unique electrical and optical properties like electron transport, thermal, chemical stability, and suitable bandgap for solar spectrum light absorption. To enhance the charge transport and photo-absorption properties of ZnO thin films, it was doped with the N^+ ion with the ion beam fluence 1×10^{15} ions/cm^2. Herein, we investigated the structural, optical and charge carrier dynamics of pristine and N^+ ion implanted ZnO thin films. We noticed the change in crystallite size and crystallinity of the samples post beam irradiation. The photo-absorption of the samples was enhanced by N^+ ion implantation with a little change in the bandgap energy. The increased Urbach energy of the ion beam irradiated sample confirms the increase disorder in its structure. Electrodes surface morphology was studied using FE-SEM which shows an increase in void spacing. Further, we performed Electrochemical Impedance Spectroscopy (EIS) to study the electrical properties of pristine and ion beam irradiated samples. The variation of real part of impedance (Z') with frequency shows a significant decrement in impedance which suggests an improved charge carrier conduction in the ion implanted ZnO thin film over the broad the frequency range (0.1 Hz to 1 MHz). The ion implantation caused the change in dielectric relaxation behaviour of the sample. M"/Mmax scaled spectra shows the sample follows non-Debye type charge carrier relaxation and multiple relaxation involved upon irradiation. This study is helpful in optimizing the ZnO based devices in applications such as sensors, charge transportation layers.

ACKNOWLEDGMENTS

We acknowledge Ministry of Education (MoE), Government of India for providing the financial support to carry this research work. We thank Mr. Rajkumar, working at IUAC, New Delhi, for providing us ion beam facility.

Analysis of Interaction of Liposomes and Nanopillar Array

Takeshi Ito*

Kansai University (Japan)

* t.ito@kansai-u.ac.jp

Abstract ID #EN-0542

Bacterial death on nanostructures has sparked great interest because the principle behind this phenomenon completely differs from that of conventional chemical antimicrobial agents [1,2]. Physical interactions between the bacterial envelope and nanostructures generate forces that deform the cell membrane. Eventually, the cell envelope breaks, causing the cytoplasm to leak out. However, the events occurring between these stages are unclear. Some paper reported that the mnbrane deformed but pilllars did not piece the cell [3]. In this work, we used liposomes as pseudo-cells because they are composed of a lipid bilayer, which is similar to a cytoplasmic membrane. We monitored time-dependent changes in the fluorescence intensities of rhodamine 6G (R6G)-containing liposomes and electrochemical impedance spectroscopy to confirm the adhesion of liposome to the surface [4]. We fabricated nanopillar array electrode composed of Au using EB lithography and pulsed wet plating. As the results, fluorescent intensity did not decreased after the adhesion. This result indicate that bactericidal property is due to organism's unique sesnsing mechanism to the stress.

ACKNOWLEDGMENTS

This work was partially supported by JSPS KAKENHI (Grant No. 21H01773).

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Development of Poly(3-Hydroxybutyrate) Based Biocomposites with Graphene Fillers of Various Structure for the Piezoresitive Sensors

Viktoriia Talaniuk[1 *], Marcin Godzierz[2], Urszula Szeluga[3], Grazyna Adamus[3], Wanda Sikorska[4], Yevheniia Buinova[5], Maksym Iurzhenko[5], Yevgen Mamunya[6]

[1] *Paton Institute of Electric Welding (Ukraine)*
[2] *Polish Academy of Sciences, Centre of Polymer and Carbon Materials, Curie-Skłodowskiej 34 street, 41-819 Zabrze (Poland)*
[3] *Centre of Polymer and Carbon Materials, Polish Academy of Sciences (Poland)*
[4] *Center of Polymer and Carbon Materials Sciences (Poland)*
[5] *E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine (Ukraine)*
[6] *Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine (Ukraine)*
* vika-toritalanuk@ukr.net

Abstract ID #EN-0545

Recently, continuous efforts have been focused on the development and research of improved flexible and highly sensitive sensors. Among various sensors, the piezoresistive type has been widely studied and used. Usually, composite materials based on conventional polymers and nanostructured materials are used to manufacture a number of these sensors with relevant properties to detect changes in temperature, touch, pressure, humidity and movement. The polymer used in these sensor materials are characterized by a long decomposition period, which creates a number of environmental problems, in particular with their disposal. To solve a number of these problems, there is a need to replace conventional polymers with biopolymers[1,2].

In this work, we propose biopolymer nanocomposites based on a mixture of poly(3-hydroxybutyrate) (PHB) and commercial aliphatic-aromatic copolyester (Ecoflex) filled with various graphene nanomaterials. The optimization procedure allowed to determine a PHB:Ecoflex weight ratio of 50:50 being the most promising for composites with graphene fillers. These polymer composite materials have similar physical and chemical properties to polypropylene based composites, that makes it possible to completely replace the conventional structural materials for piezoresistive sensors with biomaterials[3].

The principle idea of further research performed was to apply a relatively simple design of final sensor elements using graphene/PHB-Ecoflex composites prepared via facile solvent casting procedure without any additional processes. In this method, conductive graphene fillers of various structure, i.e. raw and oxidized multi-walled carbon nanotubes as well as graphene nanoplatelets, were introduced directly into biopolymer matrix [4,5]. The effect of structure and concentration of graphene materials dispersed in PHB/Ecoflex matrix on thermal, mechanical, and electrical properties of composites has been established. As a result, the free-standing films with semiconductor-like conductivity and good mechanical properties were obtained.

ACKNOWLEDGMENTS

Polish-Ukrainian join research project PAS-NASU between E.O. Paton Electric Welding Ukraine and Centre of Polymer and Carbon Materials Polish Academy of Sciences "Processing and welding new functionalized biopolymer materials"

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Electrochemical Behavior of Cobalt-Based Nanostructured Amorphous Alloys in Alkaline Solution

Mariia Lopachak[1 *], Lidiya Boichyshyn[1], Viktor Nosenko[2]

[1] *Ivan Franko National University of Lviv (Ukraine)*
[2] *G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine (Ukraine)*
* Mariia.Lopachak@lnu.edu.ua

Abstract ID #EN-0659

Amorphous metal alloys (AMAs), also known as metallic glasses, have unique properties due to their disordered atomic structure, lacking defects typically found in crystalline metals. Cobalt-based AMAs offer exceptional mechanical properties and high resistance to corrosion, making them ideal for use in harsh environments. Studying their transformation to a nanocrystalline state is important for tailoring their properties to specific applications, leading to the development of new materials with customized properties [1-3].

The process of crystallization of AMAs, including $Co_{72}Fe_5Si_{11}B_{12}$, was investigated by the method of differential scanning calorimetry. It was established that at heating rates of 10 K/min, the formation of three exothermic peaks is observed, the first of which corresponds to the process of nanocrystallization of AMA in the temperature range from 773 to 807 (±5) K. $Co_{72}Fe_5Si_{11}B_{12}$ was non-isothermally annealed at a heating rate of 10 K/min to the temperatures of nanocrystallization processes T_1 = 773K, T_2 = 787K, T_3 = 807 K where T_1, T_2, T_3 are the temperature of nucleation, growth and aggregation of nanocrystals. The X-ray diffraction method confirmed the presence of clusters and nanocrystals in amorphous structures of alloy.

To study the corrosion resistance of the nanostructured AMAs tape, cyclic voltammetry method was used in potentiodynamic mode with an automatic time scan within the potentials range of -1.4 to -0.4 V at a potential sweep rate of 50 mV/s. Based on the obtained data, the corresponding polarization curves were constructed, which served as a basis for studying the features of electrochemical processes on the surfaces of the investigated materials in a 1 M solution of KOH. It was found that the corrosion potential after annealing $Co_{72}Fe_5Si_{11}B_{12}$ shifts to the anodic side from -0,84 V to -0.45 V, which indicates an increase in the thermodynamic stability of the surface due to formed phases. In addition, the corrosion current density has decreased by 10 times and is 5×10^{-8}A/cm^2. The morphological stability of the AMA surface can be inferred from the calculated values of coefficient *a* in the Tafel equation.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Education and Science of Ukraine (award number: 0123U101830).

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Electrochemical Synthesis of Nickel-Rhenium Alloys

Oksana Bersirova[1, 2 *]

[1] *Vilnius University (Lithuania)*
[2] *V.Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine (Ukraine)*
* bersibol@ukr.net

Abstract ID #EN-0709

The rhenium alloys with nickel are promising materials with numerous useful properties: high mechanical and magnetic characteristics, microhardness, wear and corrosion resistances, and improved electrocatalytic properties. The development of new methods for the synthesis of Ni-Re alloys is of particular interest. Electrodeposition produces nanocrystalline materials when electrocrystallization results in massive nucleation and reduced grain growth. Electrodeposition is one of the most promising techniques for producing nanostructure materials owing to its low cost. However, problems related with intensification of electrodeposition and convenient control of Ni-Re alloys still limit the larger application.

It is important to establish the relationships between the kinetics of codeposition of the metals (Re and Ni) in the alloy and its composition, structure, and corrosion properties. In order to produce Ni-Re alloys, we can use stable nontoxic electrolytes. We have proposed sulfamate and citrate bath of Re-Ni electrodeposition [1,2]. The mechanism (induced and classic) of electrochemical synthesis of nickel-rhenium alloys in this electrolytes was studied [2]. The composition, structure and morphology of the Ni-Re deposits obtained depend on the composition of the electrolyte and the modes of electrolysis. Ni-Re containing over 90 at.% of Re are deposited from citrate electrolytes; the use of sulfamate electrolyte allows to increase the current efficiency (from 20 to 90%), but simultaneously the Re content is reduced (60 at.%). The effect of complexation on the efficiency of precipitation is considered. Changing the complex composition of the electrolyte and hydrodynamic conditions allows to vary the chemical composition and size of Ni-Re crystallites. As the fraction of rhenium in the deposit increases, the grain size decreases and the corrosion resistance becomes lower. As temperature increases, the Re content of the alloy from a sulfamate electrolyte decreases. It is shown that the structure of the alloys is nanocrystalline.

Analysis of the electronic configuration of metals shows that the highest catalytic effect on the hydrogen evolution reaction (HER) should be observed when one metal has d4-d5-, and another d6-d8-electron configuration [3,4]. Therefore, rhenium alloys exhibit electrocatalytic properties in the reaction of hydrogen evolution [5].

As corrosive, electrocatalytic and mechanic properties of coatings depend not only on chemical, but also on phase composition, these characteristics in this study were analyzed as a function of composition and structure of obtained Re-alloys.

ACKNOWLEDGMENTS

This research has received funding through the MSCA4Ukraine project, which is funded by the European Union (Project No. 1233494).

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Influence of Overvoltage During Electrodeposition of Thin Zn-Ni-Cu Alloy Films on its Phase Composition

Anastasiia Khomenko, Igor Ryshchenko, Antonina Maizelis*

National Technical University – «Kharkiv Polytechnic Institute» (Ukraine)

* a.maizelis@gmail.com

Abstract ID #EN-0736

Cu-Ni-Zn alloy coatings are proposed for protection steel products from corrosion as more corrosion resistant than Zn-Ni alloy [1]. It is effective for reduction of sulphate reducing bacterial survival [2]. Ni-rich surfaces of Zn-Cu-Ni electrodes are produced by chemical and electrochemical dealloying to obtain electrode materials that are catalytically active in the reaction of glucose oxidation [3], nitrate reduction [4], and hydrogen evolution during alkaline water electrolysis [5].

Alloy-based multilayer coatings have improved properties compared to single-layer coatings of constituent alloys. The properties of the alloys largely depend on their phase composition, which, in turn, depends on the electrodeposition conditions.

The aim of the study is to reveal the change in the phase composition of Cu-Ni-Zn alloy films in a wide range of potential values and current density of deposition from an ammonium glycinate electrolyte for the subsequent design of multilayer coatings based on this alloy.

Thin films of the Cu-Ni-Zn alloy 50–300 nm thick were deposited from a weakly alkaline ammonium-glycinate electrolyte. Two series of films were obtained: those deposited by the galvanostatic method and those deposited by the potentiostatic method. Cyclic voltammograms (CV) in this electrolyte, obtained on platinum, have two cathodic limiting currents associated with diffusion limitations for copper and zinc ions. The anodic branch of the CV has 2 peaks of zinc dissolution from zinc-rich phases and a multiplet peak of dissolution of α-phase of solid solution of zinc and nickel in copper, both the original and the residue from the dissolution of phases enriched in zinc. Different phases of the alloy are more selectively oxidized on anode in a more alkaline ammonia-glycinate electrolyte that does not contain metal ions. Using anodic stripping voltammetry in this electrolyte, it was revealed that copper is deposited during potentiostatic film deposition at a low overvoltage. An increase in polarization during deposition is accompanied by an increase in the fraction of the γ-phase of Zn-Ni alloy in the films, and in the fraction of nickel-enriched phase (at higher overvoltage). Films deposited under galvanostatic conditions, also contain predominantly the γ-phase in a wide range of current densities, but they are more copper-enriched as compared with films obtained at a constant potential corresponding to that established during galvanostatic deposition.

The studies have shown that it is possible to obtain Cu-Ni-Zn alloy films in an ammonium-glycinate electrolyte, containing not only predominantly the γ-phase, but also enriched in zinc, copper, or nickel, which is promising for the formation of multilayer coatings using mono-bath technique.

ACKNOWLEDGMENTS

This research is partly supported by funding from the Ministry of Education and Science of Ukraine (grant number 0123U100316).

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Metal - Organic Framework Composites for Hydrogen Energy Applications: Advances and Challenges

Kwena Desmond Modibane *

University of Limpopo (South Africa)

* kwena.modibane@ul.ac.za

Abstract ID #EN-0739

Metal-organic frameworks (MOFs) are known as porous coordination polymers, made of metal clusters and organic linkers through coordination bonds. Their structural diversity and tailorability as well as high specific surface area have made them highly advanced and multipurpose materials with applications such as green hydrogen production, water treatment, water harvesting, gas sensor, carbon dioxide capture, solar cells and battery-type energy storage. However, poor conductivity and low stability limit the capability of these MOFs. To deal with these shortcomings, fusion with the secondary components is a feasible option. Herein, efforts have been made to summarize recent research activities made at University of Limpopo, South Africa, in the synthesis of MOF composites and their hydrogen production applications [1,2]. The performance of the proposed electrolytic system for electrochemical hydrogen generation showed a huge increment of H2 production in the Palladinized graphene oxide-MOF composite induced coupling of Volmer and Heyrovsky mechanisms, for the amplification of the electrocatalytic efficiency of hydrogen evolution reaction (HER). We also reported on a simple in situ chemical oxidative polymerization of aniline in the presence of molybdenum disulphide and metal organic framework to fabricate MoS/MOF/PANI ternary composite as a precious group metal-free electrocatalysts that showed to have a good electrocatalytic grey and green hydrogen production. Furthermore, considering the cost-effective preparation of metal-organic frameworks from polyethylene terephthalate (PET) waste and their promising potential as adsorbents, this work also reports on the functionalization of PET derived-MIL-101 (Cr) with ethylenediamine (ED) for the removal of palladium ions Pd (II) from aqueous environment and photoelectrochemical hydrogen generation of the resultant composites.

ACKNOWLEDGMENTS

The authors would like to thank the National Research Foundation (NRF) South Africa for supporting and funding this research.

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The Protective Performances of Eco-friendly Zeolite Pigments for Corrosion-Resistant Paint Coatings

Mariia-Olena Danyliak*, Olha Khlopyk, Ivan Zin, Sergiy Korniy, Myroslav Holovchuk

Karpenko Physico-Mechanical Institute of the National Academy of Sciences of Ukraine (Ukraine)

* danyliak-olena@ukr.net

Abstract ID #EN-0749

Eco-friendly pigments based on synthetic zeolite for corrosion-resistant paint coatings were obtained by ion exchange method. The corrosion resistance of low-alloy steel in 0.1% NaCl solution with and without modified zeolite was investigated by potentiodynamic polarization and electrochemical impedance spectroscopy methods. It is shown that the use of zeolite modified by cations of divalent metals causes to reduce steel corrosion currents. It was established that the zeolite modified by zinc cations exhibits the most anticorrosion effect for low-alloy steel, as indicated by the values of corrosion currents, which are ~ 2 times less than one in solution without pigment. The surface morphology of low-alloy steel after immersion in neutral environment was determined by scanning electron microscopy and the formation of a protective film on its surface in solution with modified zeolite was confirmed.

ACKNOWLEDGMENTS

The work was performed within the project No. 2020.02/0063 "Synthesis and properties of new complex anti-corrosion pigments for paint coatings based on aluminosilicate nanocontainers" of the National Research Foundation of Ukraine.

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Synthesis of Water-Stable MoS_2-Tb-MoF Based Nanocomposite for Highly Sensitive Electrochemical Detection of Anthrax Biomarker Dipicolinic Acid (DPA)

Gurjeet Kaur[1 *], Saloni Sharma[1], Manoj Nayak Kumar[2], Akash Deep[3]

[1] *AcSIR, CSIR-CSIO,Chandigarh (India)*
[2] *CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C Chandigarh (India)*
[3] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India (India)*
* gurjeetkaurhera@gmail.com

Abstract ID #EN-0788

Being highly infectious to human beings and animals, dipicolinic acid (DPA), a special biomarker of Bacillus anthracis, needs to be monitored qualitatively. Herein, we designed a novel electrode modified material based on molybdenum disulfide nanoparticles and water-stable Terbium-metal organic framework (MoS_2-Tb MOF) nanocomposite for the detection of DPA. The nanocomposite has been characterized by FE-SEM, HR-TEM and elemental analysis, FTIR and the purity was further confirmed by powder X-ray diffraction (PXRD) analysis. The obtained MoS_2-based nanocomposite exhibited excellent electrocatalytic ability which could be utilized to construct an electrochemical detection platform for detecting DPA [1-3]. The electrochemical studies investigated by cyclic voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS) showed that nanocomposite could detect DPA with high selectivity and sensitivity under the optimum experimental conditions. As a result, the presented MoS_2-Tb MOF nanocomposite has good performance for detecting DPA in trace amounts suggesting its potential applications in disease prevention and environmental analysis.

ACKNOWLEDGMENTS

The authors would like to acknowledge the research fellowships provided by CSIR-CSIO India. This research work was conducted by the project grant funded by CSIR-CSIO Chandigarh under project GAP-0397. In addition, the authors are very thankful to the Director of CSIR-CSIO, Chandigarh for providing all the necessary facilities.

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TRACK 3

“MULTIFUNCTIONAL THIN FILMS & COATINGS”

Multilayer Nanoscale WN/NbN Coatings with Superior Mechanical Properties and Wear Performance

Kateryna Smyrnova[1*], Martin Sahul[2], Marián Haršáni[3], Alexander Pogrebnjak[4, 5], Lubomír Čaplovič6, Vyacheslav Beresnev[7], Mária Čaplovičová[6], Martin Kusy[5]
[1] *Slovak University of Technology in Bratislava (Slovakia)*
[2] *Faculty of Materials Science and Technology, Slovak University of Technology in Bratislava (Slovakia)*
[3] *Staton, s.r.o. (Slovakia)*
[4] *Sumy State University (Ukraine)*
[5] *Faculty of Material Science and Technology in Trnava, Slovak University of Technology in Bratislava, Trnava (Slovakia)*
[6] *Slovak University of Technology (Slovakia)*
[7] *V.N. Karazin Kharkiv National University, 4, Svoboby Sq., 61000 Kharkiv (Ukraine)*
* kateryna.smyrnova@stuba.sk

Abstract ID #MTFC-0468

The rapid development of the mechanical manufacturing industry contributes to the emergence of new materials with unique properties that could provide a reduction in economic costs and harmful environmental impacts. Particularly, the automotive and aerospace industries make extensive use of different types of cutting tools for machining expensive components. It is necessary to improve the productivity of cutting tools operating under extreme conditions and prolong their lifespan. This can be achieved by applying a hard coating on the tool surface that is designed to protect the latter from degradation. Such coatings are expected to possess high hardness, wear resistance, and low friction coefficient. Among different types of coatings, multilayer nitrides are particularly promising. A combination of two materials endows the ultimate nanolaminate with enhanced properties. The present study is focused on synthesizing multilayer coatings that consist of alternating tungsten nitride and niobium nitride nanoscale layers.

The WN/NbN coatings were deposited on stainless steel substrates by cathodic-arc evaporation (CA-PVD) using a modernized "Bultat-6" device. The substrates were biased to -50 V, -100 V, and -200 V. The effect of the negative bias voltage on the phase and chemical composition, surface roughness, cross-sectional morphology, microstructure, mechanical properties, and wear resistance of WN/NbN multilayers was comprehensively studied by grazing incidence X-ray diffraction (GI-XRD), scanning electron microscopy (SEM), wave dispersive X-ray spectroscopy (WDS), transmission electron microscopy (TEM), scanning laser confocal microscopy (LSCM), Nanoindentation and Ball-on-disc testers.

The total thickness decreased from 4.9 to 3.6 μm with an increase in Us that could be explained by respattering due to the high energies of bombarding ions. The bilayer periods (Λ) followed the same trend: coatings deposited at -50 V showed Λ of 13 nm while applying -200 V resulted in a reduction in Λ to 9.5 nm. The GI-XRD and TEM analyses revealed that all multilayers had polycrystalline structures with similar phase compositions. WN layer consisted of a face-centered cubic (fcc) β-W2N phase. The NbN layer developed a more complex structure represented by fcc δ-NbN and hexagonal ε-NbN phases. The calculated average crystallite sizes slightly decreased for all phases from approximately 2.3 to 5.0 nm. The mechanical properties were the best in the case of coating deposited at the lowest Us (hardness of 35.2 ± 3.3 GPa, elastic recovery of 55 %, H/E and H3/E2, indicating fracture toughness and resistance to deformation, were about 0.085 and 0.254, respectively). Similarly, the highest wear resistance was observed for the multilayer deposited at -50 V (friction coefficient of 0.73 and specific wear rate of about 1.01 · 10-6 mm3/N·m). The combination of all these findings makes new CA-PVD WN/NbN coatings suitable candidates for protecting cuttings tools.

ACKNOWLEDGMENTS

This research was funded by the Ministry of Education and Science of Ukraine within the General call Slovakia - Ukraine 2021 with grant number SK-UA-21-0032, and the Ministry of Education, Science, Research and Sport of the Slovak Republic with grant number 09I03-03-V01-00027. It was also supported by the Erasmus+ ICM 2020 program, project code 2020-1-SK01-KA107-078196.

About Some Physical Aspects of the Correct Representation for the State of a Nano-Scale Film

Andrii Sizhuk[1*], Yevgen Oberemok[2], Sergey Savenkov[3], Xiaohong Chen[4], Zhenjie Zhao[4], Zhuo Sun[4], Volodymyr Y Malyshev[1], Oleksandr V Prokopenko[5], Tatyana Rodionova[1]

[1] *Institute of High Technologies Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *Radiophysics Department Taras Shevchenko National University (Ukraine)*
[3] *Radiophysics Department Taras Shevchenko National University of Kyiv (Ukraine)*
[4] *Physics Department Shanghai East China Normal University (China)*
[5] *Taras Shevchenko National University of Kyiv (Ukraine)*

* andrii.sizhuk@gmail.com

Abstract ID #MTFC-0474

The process of the deposition of atoms on a substrate is commonly modeled by a most compact fulfillment of the space over the given surface, the specific symmetry of the substrate surface, the critical value of a thermodynamic free energy function, etc. The process strongly depends on the temperature of the substrate. If the atoms or molecules are deposited onto a multilayer nano-system, then the state of the new nano-layer cannot be described, strictly saying, in terms of thermodynamics, such as the temperature of the next layer. In the predefined thermodynamic limit, a macroscopic object, being in thermodynamic equilibrium with the environment, may have a minimum free energy of surface tension, which may correspond to the minimum surface of the object. Whereas a microscopic object (cluster) may have a surface energy defined as the sum of the energies of interaction between atoms (molecules) in the cluster and with the atoms of the substrate. In the latter case, the space configuration will be determined by the peculiarities of the corresponding inter-particle interaction potentials and may impose a condition of the minimum potential energy of the cluster (relative to the substrate). However, it should be remembered that, even for a system with a sufficiently large number of atoms deposited on the substrate, the condition of minimum free surface energy may not be fulfilled, since the condition of thermodynamic equilibrium, as in an isothermal process, will not be determined in principle. For example, if only the electrostatic forces of attraction between the depositing particles and the substrate dominate, we cannot speak of equilibrium processes with the minimum production rate or the maximum value of the subsystem entropy. The example of a two-layer nano-film, with a phase transition point for its reflection properties different from its macroscopic constituents, depending on the substrate temperature, is described in this work. The phase transition in the ferromagnetic-antiferromagnetic interface at temperatures higher than the Néel temperature of the antiferromagnetic is experimentally observed. The physical aspects of the correct introduction of the nano-subsystem state are discussed.

ACKNOWLEDGEMENTS

The Ministry of Education and Science of Ukraine, grant 22BF07-03

Influence of Bias Voltage on the Structure and Mechanical Properties of Dual DC Magnetron Sputtered Ti-Nb-C Films

Volodymyr Ivashchenko[1,2*], Aleksey Onoprienko[1], Alexander Pogrebnjak[3,2], Petro Scrynskyy[1], Oleksandr Marchuk[4], Andrii Kovalchenko[4], Olena Olifan[4]

[1] *Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv (Ukraine)*
[2] *Faculty of Material Science and Technology in Trnava, Slovak University of Technology in Bratislava, Trnava (Slovakia)*
[3] *Sumy State University (Ukraine)*
[4] *I.M. Frantsevich Institute for Problems of Material Science of National Academy of Science of Ukraine (Ukraine)*
* volodymyr.ivashchenko@gmail.com

Abstract ID #MTFC-0479

The films of the Ti-Nb-C system were deposited by direct current (DC) magnetron co-sputtering of composite Ti+Nb, and graphite targets onto Si substrates to which negative substrate bias in the range of –50÷–200 V was applied during film deposition. The microstructure, chemical bonds and mechanical properties of films were comparatively investigated. The X-ray diffraction (XRD) analysis revealed that the peaks of the XRD spectra of the film obtained by co-spattering of the composite Ti+Nb and graphite targets are located in intermediate region between the corresponding peaks of the Ti-C and Nb-C films. The X-ray photoelectron spectroscopy (XPS) showed that the Ti-C and Nb-C bonds prevail in the deposited Ti-Nb-C films. It was suggested that the Ti-Nb-C films are nanocomposite and consist of the crystallites of TiC-NbC solid solutions surrounded by amorphous carbon-based matrix. The Knoop hardness of the Ti-Nb-C film is highest (37.5 GPa) in the film deposited at –50 V substrate bias. The average friction coefficient determined before film delamination was the lowest (0.12) in that Ti-Nb-C film.

Structure, Hardness and Wear Resistance of Detonation Coating Based on Cr_3C_2-NiCr after Pulse-Plasma Treatment

Dauir Kakimzhanov[1*], Bauyrzhan Rakhadilov[2], Oleg Kolisnichenko[3], Yuri Tyurin[3], Dastan Buitkenov[4]
[1] *D. Serikbaev East Kazakhstan Technical University (Kazakhstan)*
[2] *PlasmaScience (Kazakhstan)*
[3] *E.O. Paton Electric Welding Institute of NAS of Ukraine (Ukraine)*
[4] *Sarsen Amanzholov East Kazakhstan University Technical University Ust-Kamenogorsk, Kazakhstan*
* dauir_97@mail.ru

Abstract ID #MTFC-0483

In this paper we investigated Cr3C2-NiCr based detonation coatings after pulsed plasma treatment. It is determined that after pulse plasma treatment (PPT) the surface roughness value decreases by 48% and the coating friction coefficient increases by 2 times, the material microhardness of Cr3C2-NiCr coatings increases from ~12 GPa (initial) to ~16.2 GPa. It was also revealed that after pulse-plasma treatment the resistance of Cr3C2-NiCr coatings to abrasion and erosion wear increases. Pulse-plasma treatment provides formation of qualitative coatings from ceramic-metal materials of Cr3C2-NiCr system with complex heterogeneous structure-phase state where the layered structure of areas of carbide particles and matrix metal in immediate proximity from border "carbide - matrix" with allocation of disperse secondary carbides in matrix is revealed.

ACKNOWLEDGMENTS

This research has been funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP09261164)

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Nano-Structuring Chalcogenide Semiconductor Thin Films with Electron Beam

Vitaliy S. Bilanych[1*], Oleg Shylenko[2], Serhii Vorobiov[3], Serhii Soroka[2], Vasyl Bilanych[1], Vasyl Rizak[1], Alexander Feher[2], Vladimir Komanicky[3]

[1] *Uzhhorod National University (Ukraine)*

[2] *Pavol Jozef Safarik University (Slovakia)*

[3] *Department of Condensed Matter Physics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, 041 54 Košice (Slovakia)*

* vitaliy.bilanych@uzhnu.edu.ua

Abstract ID #MTFC-0486

Thermoelectric materials become more and more attractive in the extensive energy consumption needs. The demand of sustainable sources such as thermoelectric generators (TEG's), and other devices allowing the conversion of heat energy into electrical power are extensively researched for energy harvesting applications [1, 2]. Due to many limitations of conventional ceramic-based thermoelectric materials (e.g. Bi_2Te_3, PbTe, $CoSb_3$) numerous development of the novel materials are directed towards flexible, light weight and low costs of polymers. One of the continuously progressing materials in electronics and nanoelectronics, biomedical devices and sensors are electrospun fibers. Electrospinning offers undoubtedly countless advantages in producing membranes, characterized with high surface area to volume ratio, with the scale up possibilities [3]. However, it is still challenging to manufacture thermoelectric electrospun fibers. Nevertheless, electrospun composite fibers with the additions of carbone- or ceramic-based fillers give wide perspective of combining thermal insulation properties of polymers and electric conductive properties, including polymer electrical conductors. Therefore, within this work the current achievements and future challenges in the field of electrospun thermoelectric fibers technology are provided. A variety of problems and current solutions are discussed, including materials, electrospun fiber's role in thermoelectric power generation, concepts of design and fabrication or thermoelectric properties and characterization methods. This study indicates the wanted and necessary strategies to develop high performance thermoelectric membranes for energy harvesting applications.

ACKNOWLEDGMENTS

This study was supported by the BioCom4SavEn project funded by the European Research Council under the European Union's Horizon 2020 Framework Programme for Research and Innovation (ERC grant agreement no. 948840) and the Polish Ministry of Science and Higher Education within the subvention funds (project no. 16.16.110.663)

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Metal-Ceramic and Epoxy Composite Materials Nanostructure Coatings

Volodymyr Korzhyk[1], Petro Stukhliak[2], Olena Berdnikova[1], Junjun Zнao[3], Kseniia Lepilina[4*], Ihor Skachkov[4]
[1] *E.O. Paton Electric Welding Institute of NAS of Ukraine (Ukraine)*
[2] *Ternopil National Technical University named after Ivan Pulyu (Ukraine)*
[3] *Scientific Research Institute of Welding Technologies named after E. O. Paton in Zhejiang Province (China)*
[4] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
*leksmih@gmail.com

Abstract ID #MTFC-0493

The usage of metal structures and various mechanisms and machines involves their operation in aggressive environments. Due to that fact their metal capacity expands, or costs increase because we need to use other metals and alloys, including those based on non-ferrous metals. However, this does not completely solve the problem of equipment usage in aggressive environments and atmospheric impact in different climate zones. One of the ways to increase the reliability of various products is the use of protective coatings. As for now scientific and technical developments offer various methods and ways of applying and forming multipurpose functional coatings. They include various composition materials gas flame spraying. Nowadays the method of cumulative-detonation multi-chamber high-speed spraying of metal powders, their oxides, nitrides, carbides, etc., has been actively developed and implemented. The advantages of this method include the high strength of adhesive joints to the base, the nanostructures formation, and the possibility of the formation of phases with different types in coating material. Metal details protective properties are improved.

The combination of metal-ceramic and polymer coatings will expand a functional range of their potential use. Gradient multi-layer coatings based on aluminum oxide and epoxy composite are proposed. The first adhesive layer is sprayed with a thickness of 100-150 microns from aluminum oxide (Al2O3) with a dispersion of 5-15 microns. Aluminum oxide is more preferable when applied to an aluminum base. Such a layer has high electrical breakdown strength, thermal conductivity and adhesive strength due to the crystalline compatibility between the aluminum base and the material of the sprayed layer. In addition, nanostructured formations appear in the coating material during spraying. It gives a wide range of required coatings operational characteristics.

Then stage a second layer of aluminum oxide with a thickness of 200-250 microns and a dispersion of 60-150 microns is successively applied. It should be noted that the porosity of the first layer is less than 0.5%. The second layer is sprayed with the set roughness parameters and the controlled number of pores in the volume of the material of the specified value is 5-20%. The third electrical insulating layer is produced with a composite containing an epoxy dian binder (100 wt. parts) brand SYD128 (China, analogue in Ukraine - brand ED -20), aluminum oxide (Al2O3) with a dispersion of 10-20 μm (10-20 parts by weight) and nanodispersed aluminum oxide with a dispersion of 100 nm (0.5-1.0 parts by weight). The third layer has the increased electrical insulation resistance to electrical breakdown (10-20 times greater than the requirements for outdoor work) and is 80-120 KV per one millimeter of coating thickness. The proposed system of gradient coatings can be used for the manufacture of structures of flat resistive heating elements.

Shaping the Band Structure of N-Type Cs_2SNi_6 Thin Films using Electron Spectroscopy

Anjana Nair V J[1], Deepa Kummattummal Govindan[2*]
[1] *Department of Physics, University of Kerala (India)*
[2] *University of Kerala (India)*

* deepachaithanya@gmail.com

Abstract ID #MTFC-0513

Perovskite solar cells have made a new revolution in the area of solar cells with its competency in achieving higher efficiencies at low manufacturing costs. The major challenge in the extensive usage of perovskite solar cell is the instability of the hybrid perovskite and the usage of lead as one of the constituent materials in the high efficiency solar cells. Vacancy ordered double perovskites with better stability and eco-friendly composition are emerged in the recent years as a solution for this. Cs_2SnI_6 is one of the emerging materials in this group having a bandgap of ~ 1.48 eV. In this work, thin films of Cs_2SnI_6 are prepared using co-evaporation method in vacuum conditions followed by thermal treatment under iodine atmosphere. Cubic double perovskite structured n-type Cs_2SnI_6 having a grain size of 0.4 mm is obtained through this process. Polygon shaped surface morphology is observed in the films.

The electronic band structure of the material is determined using a combination of different electron spectroscopic techniques, viz reflection energy loss spectroscopy (REELS), ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS). In REELS, some of the high energy incident electrons undergo inelastic interaction with the sample surface and this loss peak will appear in the spectrum. The bandgap of Cs_2SnI_6 thin film is calculated by extrapolating the onset of the loss peak which give a value of 1.5 eV [1]. The work function and valence band maximum are estimated to be 4.9 and 6.31 eV respectively from ultraviolet photoelectron spectroscopy (UPS). The core elements and their oxidation states are identified using X-ray photoelectron spectroscopy which confirms the purity of Cs_2SnI_6 phase. In addition, the valence band spectra are obtained using X-ray photoelectron spectroscopy. Here, the less bound electrons which are directly involved in the bonds between atom of the materials are considered. The experimentally obtained valence band spectra are compared with the theoretically predicted density of states. Three regions below the Fermi levels are identified in the valence band spectra, first one being comprised of energy bands due to hybridization between I p and Sn p states. The second band is due to the I p and Sn d states, the contribution from Sn d state being dominant. The top most band have contribution from all Cs, Sn, I elements and results from the mixing of d, s, and s/p/d states respectively [2]. The electronic band structure of Cs_2SnSI_6 is thus revealed with the help of electron spectroscopy.

ACKNOWLEDGMENTS

The authors acknowledge Central Laboratory for Instrumentation and Facilitation (CLIF), University of Kerala for the support to carry out the measurements. Dr.Deepa K.G. thank UGC, Government of India for the financial support offered through the UGC-BSR start-up grant (F.30-596/2021 (BSR)).

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Electrical Properties of n-NiS_2/*p*-CdTe Heterojunction Obtained by Spray Pyrolysis Method

Ivan Orletskyi, Mariya Ilashchuk, Eduard Maistruk, Ivan Koziarskyi*, Dmytro Koziarskyi
Yuriy Fedkovych Chernivtsi National University (Ukraine)
* i.koziarskyi@chnu.edu.ua

Abstract ID # MTFC-0523

Nickel disulfide (NiS_2) and cadmium telluride (CdTe) have band gaps $E_g \approx 1.3$ eV and $E_g \approx 1.5$ eV, respectively. The indicated values of Eg are in the optimal energy range for the photoelectric conversion of solar radiation energy. On n-CdTe substrates, n-NiS_2/n-CdTe isotype heterojunctions [1] with pronounced diode properties have been created by applying an n-NiS_2 film by the spray pyrolysis method, which is characterized by simple and inexpensive equipment.

The purpose of this work was to fabricate an anisotype n-NiS_2/p-CdTe heterojunction and study its electrical properties, due to the fact that anisotype heterojunctions with a p-CdTe base region and films of the electronic conductivity type in some cases [2, 3] have better electrical characteristics for practical use.

CdTe plates were cleaved from ingots obtained by the vertical Bridgman method at low Cd vapor pressure. Plates of the CdTe base material were used to fabricate n-NiS_2/p-CdTe heterojunctions. The crystals had a hole type of conductivity and kinetic parameters: electrical conductivity σ = 5.2·10-2 Ω-1·cm-1, hole concentration p = 2.1·1015 cm-3, Holl mobility μH = 55.6 cm2·V-1·s-1. The n-NiS_2 films were deposited on p-CdTe substrates by the spray pyrolysis method. Pyrolysis temperature TS = 620 K. Aerosol solutions contained $NiCl_2$·2H2O and $(NH_2)_2CS$ salts dissolved in water at a concentration of 0.1 M. The ratio [S]/[Ni] = 2.

The current rectification factor of n-NiS_2/p-CdTe heterojunctions was ~102 at |V| = 1.5 V. The contact potential difference was $\varphi k \approx 0.7$ V. The temperature coefficient dφk/dT in the temperature range T = 294 – 341 K was -2.5·10-3 eV·K-1. The forward current in n-NiS_2/p-CdTe heterojunctions is formed by tunneling of electrons from the conduction band of the NiS_2 film to the valence band of p-CdTe with the participation of surface energy levels at the interface between materials. The current through the potential barrier in the reverse bias region is determined by the generation and tunneling of charge carriers with the participation of the deep acceptor level Ev + 0.5 eV in the band gap of p-CdTe. The C-V-characteristics of the studied heterojunctions are described by phenomena that are characteristic of SIS structures with a thin $CdTeO_3$ dielectric film [4]. The presence of a dielectric determines the inversion capacitance at reverse biases. An increase in capacitance due to the accumulation of charge carriers in the valence band without limiting the capacitance by the dielectric film is observed in the C-V-characteristics at forward biases (due to the features of the energy diagram in the valence band).

The change in the inversion capacitance by an order of magnitude at high frequencies (600 kHz < f < 1000 kHz) indicates a high recombination rate of injected charge carriers in p-CdTe and contributes to the application of n-NiS_2/p-CdTe heterojunctions in high-speed electronic devices.

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Transformations in Composition and Structure in Multicomponent Alloy Targets Occurring During their Exploitation

Leonid Shaginyan[1*], Mikhail Mironov[1], Vladimir Kremenetsky[2], Vadim Novichenko[2]
[1] *Institute for Problems of Materials Science, NAS of Ukraine (Ukraine)*
[2] *Technical Center of NAS of Ukraine (Ukraine)*
* lrshag49@gmail.com

Abstract ID #MTFC-0532

The composition and microstructure of the targets used in the magnetron sputtering (MP) method may change during its operation, especially if the target is a multicomponent alloy. Therefore, the information on the composition and microstructure of the sputtered region of the target, i.e., the groove, which forms on the target over time, makes it possible to predict possible changes in the properties of the film. The targets for our experiments were fabricated from CoCrCuFeNi, CoCrCuFeMnNi and AlCoCrCuFeNiV high-entropy alloys. SEM and microanalysis were used to study the structure and composition the grooves on the targets at the beginning and at the end of their service life. The results of the investigations allowed to derive the following conclusions: 1) signs of melting found on the surface of the grooves indicate to high temperature on the targets during sputtering; 2) a new type of preferential sputtering effect has been established, the main condition of which is the presence in the target composition of microinclusions of a component whose sputtering coefficient is noticeably higher than of the others; 3) the formation of a specific microrelief on the target surface is a consequence of the combined action of two factors: high temperature and sputtering.

Electrical Properties of p-CuNiO2/n-Si Heterojunction

Dmytro Koziarskyi*, Ivan Koziarskyi, Eduard Maistruk
Yuriy Fedkovych Chernivtsi National University (Ukraine)
* d.koziarskyi@chnu.edu.ua

Abstract ID #MTFC-0547

$CuNiO_2$ belongs to a group of materials called delafossites, which are known for their wide range of electrical properties. The conductivity of these materials can vary from insulating to metallic. $CuNiO_2$ as other delafossites have good photocatalytic properties and could possibly be used for reduce water in a solar water-splitting device [1]. Copper-nickel oxide in thin film form are used as NO_2 gas sensor, anode for fuel cells, selective coating, solar cell, electrochromic devices, LEDs, photodiodes, p-type gate in heterojunction field-effect transistors, p-type transparent conductive coatings, antifungal coatings and supercapacitor coatings [2-3].

The p-$CuNiO_2$/n-Si heterostructure was obtained by radiofrequency magnetron sputtering of $CuNiO_2$ (~150 nm thick) thin films on plane-parallel n-Si plates. A stoichiometric mixture of CuO and NiO was used to make the target. This mixture was pressed into a special aluminum cup, the shape of the cup is chosen so that the plasma does not interact with the cup material. Spraying was carried out in a universal vacuum unit UVN-70, deposition process was in atmosphere of inert gas - argon. The operating frequency of the magnetron was 13.56 MHz. In order to obtain a film without impurities, a turbomolecular pump TMN-500 was used. The substrate temperature was 250 °C. The power of the magnetron was 180 W, the spraying time was 30 min. The fabrication of ohmic contacts to $CuNiO_2$ films and n-Si substrates was performed using a silver-based conductive paste. The resulting $CuNiO_2$ thin films have high resistance and transparency.

I-V-characteristics of p-$CuNiO_2$/n-Si heterostructures were measured using Arduino-based hardware and software, Agilent 34410A digital multimeter and Siglent SPD3303X programmable power supply, which were controlled by a personal computer using software created by the authors in the LabView environment. Light I-V-characteristics were measured under integrated light under standard lighting conditions close to AM1.5, and with lighting power density of 80 mW/cm2.

The research of I-V-characteristics was carried out in the temperature range of 297-344 K. Anisotypic p-$CuNiO_2$/n-Si heterostructure has a current rectification ratio RR ~ 105. The diode characteristics of the heterostructure are due to the energy barrier qφk ~ 1.7 eV. At forward biases of in the structure of p-$CuNiO_2$/n-Si the tunnel mechanism of current transfer from energy level ~ 0.19 eV prevails. The reverse current at biases $-0.9\ V < V < -3kT/q\ V$ is determined by generation mechanism of current transfer. The reverse current at biases $-3\ V < V < -0.9\ V$ is determined by tunneling processes. The p-$CuNiO_2$/n-Si heterostructure is photosensitive at reverse biases under AM1.5 radiation conditions.

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Silver Nanoparticles Entrapped in Zein Films as Biocompatible Coatings for Food Preservation

Antonica Valeria Montefusco[1*], Margherita Izzi[2], Maria Chiara Sportelli[2], Rosaria Anna Picca[2], Nicola Cioffi[2]

[1] *Department of Electrical and Information Engineering, Polytechnic of Bari (Italy)*
[2] *Department of Chemistry, University of Bari Aldo Moro and CSGI (Center for Colloid and Surface Science) – Unit of Bari (Italy)*

*a.montefusco@phd.poliba.it

Abstract ID #MTFC-0584

One of the main causes of large food losses is the cross-contamination of pathogenic microorganisms: Salmonella enterica and Listeria monocytogenes. Contamination is strictly connected to food processing lines, production lines and packaging [1]. In fact, it is required to find advanced systems able to deal with the problem [1]. To this aim, several studies and strategies are constantly proposed by the scientific community. One strategy is to develop release-based antimicrobial coatings, for example entrapping antimicrobial nanomaterials in biodegradable films.

Considering the well-known antimicrobial and anti-odor properties of silver nanoparticles (AgNPs) [2] and excellent filming properties of zein [3], in the present study we propose new coatings combining both components for the development of biodegradable and sustainable food packaging. Zein is a protein from corn, which has good hydrophobicity, and is a barrier material against humidity and gases [3]. AgNPs were prepared through a reduction process using a low amount of silver precursor, near ambient temperature for synthesis, and GRAS (generally recognized as safe) substances [4] as reducing agent (ascorbic acid) and stabilizer (citrate) [5]. As-prepared AgNPs were then properly added to zein solutions in order to obtain self-standing antimicrobial films. Transmission electron microscopy (TEM) images suggested a spheroidal morphology of AgNPs and an average size of about 30 nm. FTIR, XPS characterizations were carried out to investigate Ag loading into the films. The release of antimicrobial Ag ions was analyzed by electrothermal atomic absorption spectroscopy (ETAAS). Preliminary microbiological tests on the antimicrobial efficacy of the proposed films were performed. The perspective is to use these films as coatings for surfaces in real cases within the food industries.

ACKNOWLEDGMENTS

A.V. Montefusco acknowledges funding by European Union –NextGenerationEU – NRRP Mission 4, Component 1. ProFood-IV Prodotti e processi innovativi per la filiera ortofrutticola della IV gamma (ARS01_00755) PON Ricerca e Innovazione 2014-2020 ASSE II - Azione II.2 project is acknowledged for funding.

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Phase Composition and Structure of Ultrathin Nanocrystalline Cu-Ni Film Alloys

Valeriy B. Loboda[1*], Vladislav Zubko[1], Svitlana Khursenko[1], Vladimir Kravchenko[1], Andrey Chepizhnyi[1], Andrey Pastushenko[2]

[1] *Engineering-Technological Department Sumy National Agrarian University (Ukraine)*

[2] *Separated Subdivision of National University of Life and Environmental Sciences of Ukraine «Berezhany Agrotechnical Institute» (Ukraine)*

* loboda-v@i.ua

Abstract ID #MTFC-0585

The abstract is devoted to the study of morphology, crystal structure and phase composition of thin-film Cu-Ni alloys. Films with thicknesses up to d = 10 nm and concentrations 0 < Cu < 100 at.% were obtained in a VUP-5M vacuum unit at a residual gas pressure of ~10-4 Pa and room temperature (300 K) of the substrate by the method of separate simultaneous evaporation of the components . The resistive heating method was used to evaporate Cu, and the electron-beam method was used to evaporate Ni. The films condensed at a rate $\omega \geqslant 1$ nm/s. NaCl cleavages with a thin layer of carbon were used as substrates for electron microscopic studies (to eliminate the orienting effect of a single-crystal substrate). The film thickness was measured by the microinterferometric method with an error of 5-10%. The concentration of the film alloy components was determined by X-ray microanalysis. Electron microscopic and electron diffraction studies were carried out using a PEM-100-01 electron microscope.

The resulting ultrathin alloy films have an fcc lattice with a parameter from a = 0.352 nm to a = 0.362 nm, depending on the concentration of the components. The formation of the fcc alloy occurs already at the stage of condensation, which is confirmed by electron diffraction. It's noted that the lattice parameter in films is somewhat larger than in bulk samples. This increase can be explained both by the infiltration of atoms from the residual atmosphere into the crystal lattice of the alloy, and by the fact that the atoms of one of the alloy components during condensation can occupy positions that do not correspond to an ordered alloy.

The investigated ultrathin samples of the Cu-Ni alloy are islands, with the sizes of individual islands 0.5-2 nm in the unannealed state and up to 20 nm in the annealed state, depending on the thickness of the sample. For them, the crystal lattice parameter is 0.002-0.003 nm smaller compared to bulk samples. There are a large number of experimental works in the literature, where it is shown that in island films of pure fcc metals, depending on the conditions of preparation, the lattice parameter can be either smaller or larger compared to the lattice parameter of bulk metal, increasing or decreasing with increasing island size. However, under conditions where the influence of gas impurities is minimized, the lattice parameter always decreases with decreasing particle size.

Application of Acoustic Emission Testing to Evaluate Properties of Al-Ti-N Coatings

Ivana Sara Skrobakova*
Faculty of Material Science and Technology in Trnava, Slovak University of Technology in Bratislava, Trnava (Slovakia)
* ivana.skrobakova@stuba.sk

Abstract ID #MTFC-0593

The coatings are widely used in various applications as they can provide better properties, such as higher hardness, wear and oxidation resistance, etc. Their ongoing development allows usage of nano-structure materials to reach specific and unique properties. Our study is related to of AlTiN coatings deposited with various chemical composition and deposition parameters on an industrial hard coating unit- PLATIT π80 +DLC on high-speed steel substrate and their adhesion evaluation. For this reason, we used new method of adding acoustic emission measurement along with indentation measurements. The results were compared according to VDI 3198 Indentation test standards to show the possibility of application of AE as appropriate method to detect even cracks creation or other damage within the material.

Electrodeposition in a Magnetic Field of Electrocatalytically Active and Ferromagnetic Alloys

Yuliya Yapontseva[1], Valeriy Kublanovsky[1*], Tetyana Maltseva[1], Oksana Gorobets[2]
[1] *V.Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine (Ukraine)*
[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
* kublan@ukr.net

Abstract ID #MTFC-0600

A study and mathematical modeling of the influence of a constant magnetic field on the electrodeposition of refractory metals (molybdenum and rhenium) alloys with cobalt from monoligand citrate (pH 3.5) and polyligand citrate-pyrophosphate (pH 9.0) electrolytes were carried out. It is shown that, in addition to standard methods for controlling electrochemical processes (changing the current density, temperature, ratio of components in solution and hydrodynamic regime) for coatings exhibiting electrocatalytic activity in the hydrogen evolution reaction and ferromagnetic coatings, one of the most promising ways to influence the composition and structure is electrodeposition in a constant magnetic field.

It has been found that the use of electrolytes of various complex compositions makes it possible to deposit alloys containing refractory metals in a wide range, especially in the case of rhenium alloys. Deposition in a magnetic field makes it possible to obtain less stressed coatings and, in the case of rhenium alloys, to halve the crystallite size. The magnetic properties of the obtained coatings depend on the refractory metal nature and by choosing the refractory metal and its content in the alloy it is possible to control the properties of the coatings in a wide range from softmagnetic to hardmagnetic .

The ways of the magnetic field influence on the CoRe and CoMo alloys electrodeposition, the reasons for the formation and intensity of convective flows, as well as the influence of the parallel process of gas evolution and the coatings magnetic properties are shown by the mathematical modeling method.

The conducted studies prove the feasibility and prospects of magnetoelectrolysis use to improve the quality and intensify the process of coatings electroplating of refractory metals alloys with iron group metals, as well as improved the understanding of the mechanism of action of constant and gradient magnetic fields on multistage electrochemical processes.

The Influence of Plasma Treatment on Thermal, Dynamic-Mechanical and Rheological Properties of Polymeric Material

Silvia Ďurišová*, Mariana Pajtášová, Róbert Janík, Katarína Moricová, Ivan Labaj
Alexander Dubček University of Trenčín, Faculty of Industrial Technologies in Púchov (Slovakia)
* silvia.durisova@tnuni.sk

Abstract ID #MTFC-0602

Recently, the plasma treatment of polymeric materials has become a sufficient way of surface properties modification within a huge range of its application. Typically, different plasma sources affect the structural properties, morphology and wetting characteristics of polymeric materials.

However, the presented work is focused on the characterization of plasma modified polymeric composite material by thermal analysis performed via differential scanning calorimetry and thermogravimetry in oxygen and nitrogen atmosphere. Within this study was used plasma reactor based on diffuse coplanar surface barrier discharge working in artificial air at power of 375 W. The examined exposure time was set on 10 s. Also, the active plasma distance from sample surface was evaluated. Secondly, the effect of plasma modification was aimed at the characterization of elastic modulus and loss modulus within the range of temperature from -70 °C to 70 °C at a frequency of 1kHz. Also, the rheology parameters aimed at the mentioned modulus comparison were monitored. Additionally, the effect of plasma was studied via curing properties wherein curing time (tc90), scorch time (ts) and curing rate index (CRI) were measured. Furthermore, the rheometry properties, the minimum torque (ML), maximum torque (MH), Payne effect and viscosity before and after plasma treatment were studied.

ACKNOWLEDGMENTS

The authors would like to thank the Slovak Grant Agency KEGA for financial support (GRANT KEGA 001TnUAD-4/2022).

Surface Modification of Amorphous Alloys with Heterofunctional Oligoperoxide Metallic Complexes

Oksana Myronivna Hertsyk[1*], Tetiana Heorhiivna Hula[1], Myroslava Oleksiivna Kovbuz[1], Olga Anatoliivna Ezerska[2], Myroslava Stepanivna Tashak[3]
[1] *Ivan Franko National University of Lviv (Ukraine)*
[2] *Fraunhofer Institute for Production Technology and Advanced Materials (Germany)*
[3] *Lviv National Polytechnic University (Ukraine)*
* o_hertsyk@yahoo.com

Abstract ID # MTFC - 0604

The adsorption interaction at the phase boundary determines the adhesion of oligomeric films on the surface of amorphous metallic alloys (AMA). Such films either protect the metal surface from external aggressive influences, or functionalize it in order to provide the properties of a low-temperature surface free radical initiator for covering the surface with a grafted polymer layer.

Tapes of AMAs $Fe_{78,5}Ni_{1,0}Mo_{0,5}Si_{14,0}B_{6,0}$ and $Fe_{73,1}Cu_{1,0}Nb_{3,0}Si_{15,5}B_{7,4}$ were studied.

As the main film former, an oligoperoxide metallic complex (OMC) based on vinyl acetate (VA), 2-tert-butylperoxy-2-methyl-5-hexen-3-yne (VEP) and maleic anhydride (MA) was used, which has specific properties of initiating radical low-temperature polymerization. (OMC), where Me^{m+} - $[Cu^{m+}]$ content of 0,3 та 0,85%, a L_1 і L_2 - are low-molecular ligands, which are solvent molecules used as a medium for the synthesis of OMC.

OMC films were applied to the surface of the electrodes by keeping them in 1% water-ammonia solutions of film formers for different durations. The optimal conditions for spontaneous adsorption of macromolecules on the surface of AMA were estimated by the chronopotentiometric method and the electrochemical impedance spectroscopy method.

A comparison of the films characteristics obtained from freshly prepared solutions and solutions that were kept for 90 days at a temperature of (291±2) K in the dark, showed that the investigated solutions of film formers are unstable, capable of creating intermolecular connections, which reduces their adhesion to the metallic surface.

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Development of $K_2Eu(PO_4)(WO_4)$ – based Luminescent Phospho-Tungstate Glass-Ceramics

Vitalii Chornii[1,2*], Volodymyr Boyko[1], Maksym Lazarenko[2], Mykola Slobodyanyk[2], Serhii Nedilko[2,3], Kateryna Terebilenko[2], Petro Teselko[2], Valeriia Zozulia[2], Yaroslav Zhydachevskyy[3], Andrzej Suchocki[3]
[1] *National University of Life and Environmental Sciences of Ukraine (Ukraine)*
[2] *Taras Shevchenko National University of Kyiv (Ukraine)*
[3] *Institute of Physics Polish Academy of Sciences (Poland)*
* Vchornii@gmail.com

Abstract ID # MTFC-0619

Glass-ceramics (GCs) reveal better physical and chemical properties comparing to organic silicon or resins used in high power light emitting diodes (LEDs) [1]. In particular, GCs possess a higher heat conductivity and better thermal stability, resulting in lower degradation of light efficacy and consequently increased LED operation time. The glass component should have glass-transition temperature, Tg, higher than typical operation temperature in high power LEDs (T ≈ 100-200 ˚C [1]) but not as high as for silica ones (Tg ≈ 1100 ˚C [2]). Another issue to be studied is light scattering in such GCs. It must be as small as possible that can be achieved by selection of vitreous and crystalline components with close refractive indices. The phospho-tungstate glasses with phosphate and/or tungstate micro/nano-phosphors embedded give a possibility to achieve suitable Tg and low light scattering.

The glasses of the K_2O-P_2O_5-WO_3-V_2O_5 and K_2O-P_2O_5-WO_3-Bi_2O_3 compositions both pure and Eu^{3+} doped have been prepared by conventional melt quenching. The samples of GCs were obtained by co-sintering of starting glass and $K_2Eu(PO_4)(WO_4)$ micro/nanocrystalline phosphor. The samples of glass and GC have been characterized via powder X-ray powder diffraction, thermogravimetric analysis (DTA), scanning electron microscopy, energy dispersive X-ray analysis, IR, optical absorption, and photoluminescence (PL) spectroscopy.

It was found that the samples of glass-ceramics consist of glass host and embedded $K_2Eu(PO_4)(WO_4)$ particles of sizes below of 10 m. The glass transition temperature was found to be near 370 °C for all the samples based K_2O-P_2O_5-WO_3-V_2O_5 glass host. The IR spectra have shown the presence of various molecular groups, namely PO_4, P_2O_7, P4O12, WO4, WO6 and VO4 in the glass and GCs. The Eu3+ - containing samples of glass and GC reveal intensive red luminescence under excitation at 365, 405, and 473 nm at room temperature. These wavelengths correspond to maxima in PL excitation spectra and matched well with cheap UV, violet and blue light emitting semiconductor chips. The photoluminescence is related with f-f radiation transitions in the Eu^{3+} ions. The widths of some spectral lines in the GC emission spectra are comparable with ones for $K_2Eu(PO_4)(WO_4)$ crystals [3], while other lines are somewhat widened. The line widening may be ascribed to partial melting of the $K_2Eu(PO_4)(WO_4)$ crystallites accompanied with the diffusion of Eu^{3+} ions into glass host. The results obtained are discussed in terms of the interphases interaction. The developed glass-ceramics can be considered as promising luminescent materials for elaboration of light-transforming coatings for high-power white LEDs.

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Inkjet-Printed Luminesce Metal-Organic Framework Patterns as the Ammonia Gas Sensor

Priyanshu Goel*
Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India (India)
* priyanshu.goel@uni-konstanz.de

Abstract ID #MTFC-0623

Metal-organic framework (MOF) belongs to the family of highly porous materials in which Metal Ions combines with organic linker to form a 3D frame or mesh like structure [1,2]. MOF possesses astonishing properties like high stability, large surface area, and high porosity that leads to its exploration in various fields i.e., gas absorption, catalyst, sensing, and energy devices [2,3]. In the presented work, firstly a luminescent Tb-MOF ink was synthesized which was then used to fabricate the inkjet printer thin film. Secondly, these thin films were then used to sense different Volatile compounds (NH3, Ethanol, H2S, and HCL vapors) [4]. Results demonstrate that the host-guest chemistry of the MOF with Ammonia molecules quenches the luminescence of these thin films when the concentration of the ammonia was increased (5-80 ppm). Furthermore, these printed strips are reasonably sensitive with a low limit of detection of 0.3 ppm.

ACKNOWLEDGMENTS

It is with great gratitude that Priyanshu Goel acknowledges the research fellowship (Herz Fellowship 2021) provided by the University of Konstanz in Germany and CSIR-CSIO India. This was conducted by the project grant funded by CSIR-CSIO Chandigarh under project MLP-2006.In addition, for providing all the facilities necessary, the authors are very thankful to the Director of CSIR-CSIO, Chandigarh.

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Luminescent Composites Based on Nanocellulose and $K_3Tb(PO_4)_2$ Phosphor – Preparation and Properties

Serhii Nedilko[1,2*], Vitalii Chornii[3,1], Kateryna Terebilenko[1], Petro Teselko[1], Vasyl Scherbatskyi[1], Danylo Gerasymchuk[1], Artem Voinalovych[1], Volodymyr Boyko[3], Yaroslav Zhydachevskyy[2], Valerii Barbash[4], Olga Yashchenko[4]

[1] *Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *Institute of Physics Polish Academy of Sciences (Poland)*
[3] *National University of Life and Environmental Sciences of Ukraine (Ukraine)*
[4] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
*SGNedilko@gmail.com

Abstract ID #MTFC-0643

Cellulose and its derivatives have been considered as outstanding materials for flexible hybrid printed electronics. It is a rapidly growing field because it provides high throughput manufacturing of electronics that enables economies of scale, resulting in more affordable products [1]. Furthermore, a nanocellulose combines properties of natural polymer and nanomaterials resulting in wider horizons for cellulose-based materials applications, partially in optoelectronic devices [2]. The abundance of cellulose sources in nature and variety of methods determine cheapness of micro- and nanocellulose production. So, there are number of reports on the preparation of nanocellulose-based luminescent materials, their properties and applications. However, the interactions between polymer and phosphors and its impact on optical properties of such composites have been attracted little attention so far. Here we report a morphology and optical properties of nanocellulose-based thin films containing luminescent oxide.

The nanocellulose was obtained from non-wood materials (straw pulp) [3] and $K_3Tb(PO_4)_2$ in a form of micro/nanopowders was synthesized from melt. The composite films have been obtained by mixing of water suspensions of nanocellulose and the oxide. These mixtures undergo ultrasonic treatment and water evaporation in air at t = 50 ˚C. The morphology of the films has been studied by optical microscopy as well as scanning electron microscopy accompanied by energy-dispersive spectroscopy. The optical properties of the films have been studied using of DFS-12 spectrophotometer and xenon arc lamp (DXeEL-1500) accompanied by MDR-4 monochromator as excitation light source.

The obtained data on composite films properties have been analyzed together with corresponding data for starting oxide micro/nanopowders and thin film made from initial nanocellulose. It was found that visible luminescence of composite films can be excited from ultraviolet to blue spectral region. In particular, under excitation at 386 nm emission of Tb^{3+} ions (intensive bands near 545, 580 and 620 nm) dominates in spectra of composites. The nanocellulose host luminescence band with maxima near 570 nm was observed when excitation took place at 440 nm, while only weak Tb^{3+}-related emission was found for this excitation wavelength. The studied composites can be considered as luminescent substrate for printable optoelectronics devices.

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The Characteristics and Photocatalytic Activity of Lanthanum Doped ZnO Films

Liliia Myroniuk[1*], Denys Myroniuk[1], Olga Chudinovych[1], Eduard Maistruk[2], Ivan Koziarskyi[2], Olena Olifan[3], Ihor Danylenko[4], Arsenii Ievtushenko[1]

[1] *Frantsevich Institute for Problems of Materials Science, NAS of Ukraine (Ukraine)*
[2] *Yuriy Fedkovych Chernivtsi National University (Ukraine)*
[3] *I.M. Frantsevich Institute for Problems of Material Science of National Academy of Science of Ukraine (Ukraine)*
[4] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine (Ukraine)*
* liliiamolotovska@gmail.com

Abstract ID # MTFC-0679

The optical, magnetic and structural properties of ZnO can be modified by ionic doping of suitable elements. Doping of ZnO with rare earth elements provides the efficient modulation of the emission in the visible range owing to their unique optical properties. Among the rare earth elements (REE), Lanthanum (La) is efficient dopant that significantly improves the properties of ZnO such as catalytic activity, dielectric constant, and promotes the more controlled growth of high-quality thin films [1]. Furthermore, La-doped ZnO materials show excellent gas sensitivity and photocatalytic activity [2].

Present work is focused on investigating the result of La doping concentration on the structure, optical and photocatalytical properties of undoped and La-doped ZnO films.

Undoped and La-doped ZnO films were successfully sputtered by radio frequency magnetron sputtering on silicon and glass substrates using the universal vacuum unit UVN-70. Before the sputtering, the vacuum chamber was pumped to a residual pressure of 5·10-5 mm Hg. Compressed ceramic tablets of pure ZnO and ZnO:La_2O_3 5 and 10 % wt. were used as targets and were sputtered in an Ar atmosphere at a power of 200 W. Substrate temperature was establish at 350 °C. Sputtering time was 30 min.

The results of scanning electron microscopy confirmed that La is doped with ZnO. The incorporation of La cations in crystal structure of ZnO changed the morphology of ZnO films. It has been observed after an increase in the La_2O_3 doping percentage from 5 to 10 % wt. when the dendritic outgrowths had grown into well-ordered hexagonal crystals.

The analysis of X-ray diffraction pattern of undoped and La-doped ZnO films demonstrates that all films are textured polycrystalline hexagonal wurtzite structure with the prominent peak corresponding to the (002) plane. No additional peaks due to segregated La or La_2O_3 phases have been found in the films, thus indicating their high phase homogeneity which also confirms by EDX analysis. This indicates that La ions are uniformly substitute Zn in the cation sublattice of ZnO lattice. Also was found the low angle peak (002) shifting that confirms increased interplanar spacing and imply the Zn substitute on larger La ions.

The influence of La on photocatalytic activity of ZnO films will be presented and discusses in our report in detail.

ACKNOWLEDGEMENTS

This work supported by the research project of the NAS of Ukraine "Creation of promising materials based on ZnO doped REE for use in catalysis".

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Effect of Interfaces Number on the Thermally-Induced Phase Transitions in Ni/Ti Stacks

Vlad Mohylko[1], Ivan Kruhlov[1], Svitlana Voloshko[2], Andrii Orlov[1*]

[1] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
[2] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
* orlov.a.k.apeiron@gmail.com

Abstract ID # MTFC-0690

NiTi alloys are among the most widely used materials for the fabrication of microelectromechanical (MEMS) devices such as microactuators, micropumps, microdrives, etc. This is attributed to the pronounced shape-memory effect (SME) of NiTi which is due to the thermoelastic martensitic-austenitic phase transition taking place at close to room temperatures. Moreover, this effect is reversible and demonstrates a unique ability to restore inelastic deformation after removal of loads.

Thin-film NiTi materials are especially attractive for the variety of SME-based applications since they exhibit much smaller heat/cool mass compared to the bulk, which results in the higher operation rate and decreased response time. The most common approach of obtaining NiTi thin films with a composition close to equiatomic is their deposition on heated substrate using simultaneous magnetron sputtering of high-purity Ni and Ti targets. However, the precise control over the phase formation became challenging in this case due to the high sensitivity of the process to the chemical composition. Here we show that an adequate alternative approach is the synthesis of layered Ni/Ti stacks followed by their thermal annealing to induce the ordering.

We found that increasing the number of interfaces by increasing the number of Ni and Ti nanolayers, while maintaining the similar total thickness of 60 nm, leads to a shift in the temperature of the onset of solid-state reactions. This effect is related to the phenomenon of amorphization at the interfaces between metals with high lattice mismatch, which starts at 100°C lower temperature when the thickness of each layer is decreased twice. For the bi-layered Ni/Ti stack, the annealing at 400°C results in the amorphization of crystalline phases of both metals, while the similar effect is revealed for the four-layered [Ni/Ti]x2 stack after annealing at 300°C. The processes of amorphization are accompanied with the diffusion of Ti towards the outer surface and its segregation on it, which also occurs at 300°C and 400°C for the Ni/Ti and [Ni/Ti]x2 films, correspondingly. The next increase of the annealing temperature up to 600°C leads to the diffusion-induced formation of the NixTiy intermetallic phases relevant for the applications in the SME-based microdevices. Therefore, our findings demonstrate a pathway for tuning the onset temperatures of solid-state reactions in Ni/Ti structures by adjusting the number of metal nanolayers before their thermal treatment.

ACKNOWLEDGEMENTS

This study has been supported by the Ministry of Education and Science of Ukraine grant (0121U110283).

Patterning of Titanium Nitride Films by Dry Reactive Ion Etching in Inductively Coupled Plasma

Tibor Izsák[1*], Tomáš Ščepka[1], Gabriel Vanko[1], Ján Fedor[1], Oleksandr Romanyuk[2], Boris Hudec[1]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*
[2] *FZÚ - Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6 (Czech Republic)*
** tibor.izsak@savba.sk*

Abstract ID # MTFC-0695

Titanium nitride (TiN) is a key material in the semiconductor industry due to its compatibility with CMOS devices. It is characterised by many interesting properties such as high thermal stability, good electrical conductivity, including matching lattice structure and good adhesion with the high-k materials [1] (e.g. HfO_2, ZrO_2, Al_2O_3). TiN has found use in many applications such as tunable work-function metal gates in field-effect-transistors (FETs), diffusion barriers, metal hard masks, anti-reflective coatings, extreme ultraviolet patterning, sub-bandgap and Schottky photodetectors [2]. However, in order to form the FET structure of TiN gates, an etching process is required.

Various etching processes have been developed for TiN, including wet etching processes, conventional dry reactive ion etching (RIE) processes using Cl- or F-based chemistries, or plasma atomic layer etching. Wet etching processes typically exhibit high surface roughness, making it difficult to control the etch rate at the nanometre scale. Although RIE can control the etch rate with anisotropic patterns, there are many studies that contradict the etching mechanism of TiN thin films [3-5]. Another problem with TiN etching in Cl- and F-based plasmas is related to the formation of non-volatile by-products, which can degrade the properties of the final etched structures. Therefore, a thorough study is needed to optimise the etching process to achieve the required etch rate, etch profile and selectivity to the mask material.

In the present work, we have investigated the dry reactive ion etching of TiN films using an Oxford Plasmalab 100 inductively coupled plasma (ICP) system in fluorine-based chemistry. The influence of the CF_4/Ar gas mixture ratio, the effect of the ICP power, and the pressure were investigated. The etching rate and the etch profile were evaluated from surface profilometer and SEM measurements. It was found that increasing the ICP power increases the selectivity of the photoresist mask to TiN (from 0.22 to 0.63), and also improves the etch profile (~51° tilt angle for 200 W of ICP power compared to ~17° tilt angle for pure RF plasma only). The etching rate of TiN was varied from 2 to 40 nm/min. The lowest etching rate was observed for the Ar-rich RF plasma, proving the dominance of the chemical etching over the physical sputtering process. The uniformity of the etching process was also investigated. The best uniformity was achieved at 15 mTorr pressure, where the difference in etch rate measured over a 2" substrate was only ~1.2 nm/min. In addition, XPS measurements were performed on the samples in order to analyse the non-volatile by-products formed on the etched TiN structures.

ACKNOWLEDGMENTS

This work was supported by the Operational Program Integrated Infrastructure for the project: New fabrication technology of sensors, detectors and memristors for intelligent microelectronics in the 21st century, ITMS project code 313011BVN5, co-financed by the European Regional Development Fund (ERDF).

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Growth of Two-dimensional MoS_2 and WS_2 Films by Pulsed Laser Deposition on Sapphire Substrates

Marianna Španková[1*], Edmund Dobročka[1], Tatiana Vojteková[1], Béla Pécz[2], Miklós Németh[2], Peter Hutár[3], Salvatore Panasci E.4, Filippo Giannazzo[4], Stefan Chromik[1]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Centre for Energy Research, Institute of Technical Physics and Materials Science, Konkoly-Thege ut 29-33, 1121 Budapest (Hungary)*

[3] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava (Slovakia)*

[4] *CNR-IMM, Strada VIII, 5 95121, Catania (Italy)*

* *marianna.spankova@savba.sk*

Abstract ID #MTFC-0702

The distinctive electronic, mechanical, and optical properties of two-dimensional (2D) layered transition metal dichalcogenides (TMDs), such as molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2) have gained significant interest. Due to the presence of a definite bandgap, roughly 1.8 eV, 2D MoS2 has gained significant attention as a promising material in the field of optoelectronics device development. Similarly, WS2, a fellow member of 2D TMDs, shares comparable characteristics to MoS_2. WS_2 possesses superior thermal stability and optical properties.

Here we report the growth of few monolayer thick MoS_2, WS_2 and their heterosructures on c-sapphire substrates by pulsed laser deposition (PLD). This technique is a simple, highly manageable, and efficient method for large-area thin film fabrication. A KrF excimer laser operating at 248 nm with the energy of pulse 50 – 70 mJ, repetition rate 4 Hz, was used to grow the MoS_2 and WS_2 layers. The temperature of the thermocouple was set up to 860 °C. After deposition, the temperature was decreased at a rate of 50 °C/min down to 200 °C, and then by natural cooling.

The prepared films have been characterized by several techniques, including Raman spectroscopy, X-ray diffraction, scanning electron microscopy (SEM) and cross-sectional scanning transmission electron microscopy (STEM).

X-ray diffraction analyses of the MoS_2 and WS_2 films confirmed the preferential growth of the films. Raman spectroscopy verified the presence of the MoS_2 and WS_2 structure with the appearance of two distinct peaks for the E^1_{2g} and A_{1g} vibrational modes. The number of layers depends on the peak distance between the E^1_{2g} and A_{1g} modes of the films. We compared the number of monolayers obtained through Raman analysis with the results from STEM. The high-resolution image taken in TEM mode and based on the lattice spacings shows 2-3 monolayers of the MoS_2 or WS_2 grown on c-sapphire which is a good agreement with the measured Raman spectra results.

We have shown that using the PLD method we are able to prepare a few monolayer thick uniform and stoichiometric MoS_2 and WS_2 thin film which may have applications in next generation 2D electronics.

ACKNOWLEDGEMENTS

The results were achieved within the Project "ETMOS — Epitaxial Transition Metal dichalcogenides Onto wide bandgap hexagonal Semiconductors for advanced electronics". The work was also supported by the Slovak Grant Agency for Science, VEGA 2/0140/22.

Heterostructures of Diamond and Transition Metal Dichalcogenides

Marián Varga[1*], Michaela Sojkova[1], Jana Hrdá[1], Gabriel Vanko[1], Tibor Izsák[1], Martin Hulman[2,3], Michal Kočí[4], Jan Fait[4], Alexander Kromka[4]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*

[3] *Danubia NanoTech s.r.o., Bratislava (Slovakia)*

[4] *FZÚ - Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6 (Czech Republic)*

* marian.varga@savba.sk

Abstract ID #MTFC-0705

Diamond (3D) has gained a reputation as an extremely versatile material due to its unique combination of physical/chemical/electrical/optical properties which can be utilized for a wide range of applications. Equivalently, 2D transition metal dichalcogenides (TMDs) have also attracted significant attention due to their photonic/electronic properties. Besides the usage of individual forms of these materials, their combination could serve as an excellent heterostructure revealing novel phenomena and functionalities at their interface. For this reason, various technological procedures are being studied and optimized to obtain high-quality 3D/2D heterostructures, preferably on a large scale. In this work, we deal with the preparation of diamond/TMD (specifically MoS_2 and $PtSe_2$) and vice versa heterostructures using chemical vapor deposition methods. From a technological point of view, the diamond growth on TMD is a highly challenging issue with several limitations, and we will show that these can be overcome by properly chosen growth procedures. On the other hand, the TMD growth on diamond is more favourable and the fabricated TMD/diamond heterostructures, for instance, revealed improved gas sensing properties to NH_3/NO_2 gases at room temperature. In addition, based on theoretical calculations, we will discuss the fine-tuning of photonic diamond structures using TMD (multi) layer(s) on top.

ACKNOWLEDGEMENTS

This work was supported by the MoRePro project No. 19MRP0010 and funding from the Slovak Academy of Sciences.

High Aspect Ratio GaAs Structures for Improved Radiation Detectors

Tibor Izsák[1*], Gabriel Vanko[1], Eva Kováčová[1], Marian Vojs[2], Bohumír Zaťko[1]
[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*
[2] *Institute of Electronics and Photonics, Slovak University of Technology, SK-841 04 Bratislava (Slovakia)*
* tibor.izsak@savba.sk

Abstract ID #MTFC-0706

Deep etched high aspect ratio structures in GaAs are often required for MEMS applications [1], including through-vias [2], as well as for photonic [3] and solar applications. Many applications require an anisotropic etch profile with smooth sidewalls as well as a high etch rate and aspect ratio. Therefore, the fabrication process of these structures in GaAs typically requires dry-etching techniques such as reactive ion etching (RIE). The key factors in the RIE process are the use of a suitable mask material with appropriate selectivity and optimized etch conditions.

Our motivation is to fabricate high aspect ratio (>1:5) GaAs structures array (with depth of >100 µm), which will be further used for the fabrication of radiation detectors. Therefore, we have designed a two-layer etch mask system, where the top ~100 nm thick metal layer is used as an etch mask to etch the underlying SiO_2, and the thick SiO_2 layer (>3 µm) serves as an etching mask for deep GaAs etching. The SiO2 is an ideal option due to the GaAs is typically etched in a Cl-based gas chemistry, while SiO_2 is etched in a fluorine-based gas chemistry [4], thus having high selectivity to GaAs.

In the present work, we first optimized the structuring of SiO_2 film in an Oxford Plasmalab 100 inductively coupled plasma (ICP) system using different metal mask materials (Al, Cr, Ni) and variable conditions of fluorine-based plasma chemistry. It was found that the combination of CF_4/O_2/Ar in a ratio of 50/2.5/2.5 sccm at a pressure of 7 mTorr, ICP power of 500W and DC voltage/RF power of 60V/21W is sufficient to achieve high selectivity at satisfactory etching rate (~ 65 nm/min). The highest selectivity of the metal mask to the SiO_2 film was evaluated for the Ni layer (~ 70), which was 5.5x and 3.5x higher than for the Al and Cr masks, respectively. In practical terms, this means that a 100 nm thick Ni layer should be sufficient to produce a structured SiO_2 film with a maximum thickness of ~ 7 µm.

In the next step, we have studied the deep reactive ion etching of GaAs substrates in the ICP system using the above mentioned SiO_2 mask with a thickness of 2.2 µm. The effect of RF power, pressure and gas mixture ($Ar/SiCl_4$ ratio) on the etching rate and anisotropy was investigated. The best anisotropy of GaAs etching was observed for the following parameters: ICP power of 400W, RF power of 80W (at DC 300V), pressure 20 mtorr, gas mixture ratio $Ar:SiCl_4$ = 20:1, giving an etching rate of ~0.5 µm/min. SiO_2 showed relatively high selectivity to GaAs (i.e. 32-50, which means that SiO_2 with a thickness of 3-5 µm should be sufficient to obtain 120-160 µm depth etches in GaAs substrates. Preliminary results showed that further improvement is possible by reducing the ICP power and increasing the $Ar:SiCl_4$ gas mixture ratio.

ACKNOWLEDGEMENTS

This work was supported by the grant of the Slovak Research and Development Agency grant No. APVV-18-0273 and by grant of the Scientific Grant Agency of the Ministry of Education of the Slovak Republic and the Slovak Academy of Sciences No. VEGA 2/0084/20.

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Room Temperature Fabrication of Low Resistivity Titanium Nitride Thin Films by DC Magnetron Sputtering

Tomáš Ščepka[1*], Ján Fedor[1], Fridrich Egyenes[1], Marián Precner[2], Edmund Dobročka[1], Alica Rosová[1], Iuliia Vetrova[1], Boris Hudec[1]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)[3] University of Palermo (Italy)*

*tomas.scepka@savba.sk

Abstract ID #MTFC-0708

Titanium nitride (TiN) is an extremely hard material with high thermal and chemical stability and low electrical and thermal resistivity. Hence, it is used in many applications in the microelectronics industry as adhesion layer, diffusion and corrosion barrier [1], electrode material for transistor gates [2], Schottky contact, or for DRAM cells [3].

Here, we deposited TiN films by reactive sputtering using a titanium target in a N_2/Ar ambient at room temperature at different working pressures and nitrogen flow rates with the aim to obtain thermally stable TiN films with lowest resistivity patternable using lift-off technique. Resistivity is found to improve for lower working pressures while increasing nitrogen flow did not play an important role. Thermal stability was investigated by annealing at 300°C in oxygen and nitrogen atmospheres for 1h and measuring resulting resistivities, which increased for all the studied films after annealing, and more in O_2 than in N_2. TiN film with the lowest initial resistivity also showed highest thermal stability among studied films. Moreover, the roughness of the deposited films increases for higher working pressures.

ACKNOWLEDGMENTS

This work was supported by the Operational Program Integrated Infrastructure for the project: New fabrication technology of sensors, detectors and memristors for intelligent microelectronics in the 21st century, ITMS project code 313011BVN5, co-financed by the European Regional Development Fund (ERDF). Authors are thankful to Dr. Marián Mikula for fruitful discussions.

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Impact of Pulse Potential Amplitude of Substrate on the Structure and Mechanical Properties of Diamond-Like Films

Oksana Horobei[1*], Yurii Nasieka[1], Volodymyr Strelnytskyi[2]
[1] *V.E. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine (Ukraine)*
[2] *National Science Center "Kharkov Institute of Physics and Technology" (Ukraine)*
* oksanagorobey028@gmail.com

Abstract ID #MTFC-0712

Tetrahedral amorphous carbon is a promising material for the fabrication of protective and functional coatings. Similarity of this material to diamond is manifested in such characteristics as high hardness, biocompatibility, wear resistance, chemical inertness, and thermal conductivity [1, 2]. This makes diamond-like carbon (DLC) coatings an indispensable material in medicine, aerospace industry, and other applications.

This work presents the results of studies of thick (up to 5 μm) amorphous films based on diamond-like carbon with minimal surface defects. The films were deposited by vacuum arc method using a linear magnetoelectric plasma filter of the graphite cathode to remove micro-particles. The object of the study was the influence of the amplitude of the pulsed bias potential on the substrate during deposition in the range of 0-2 kV on the structure and mechanical properties of the coatings.

Mechanical characterization of the coatings were performed by the nanoindentation method as dependence of hardness and Young's module on the amplitude of the pulse potential. It was found that in the absence of pulse application, i.e. at a "floating" potential of 50 V, a diamond-like coating is formed, with a maximum volume fraction of sp3 carbon phase reaching 80%. The coating manifests high hardness and Young's modulus of 69 GPa and 496 GPa, respectively, but it is brittle and has poor adhesion to the steel substrate.

The pulses were applied with a duration of 6 μs and a frequency of 12 kHz. Application of the pulses to the substrate leads to a significant decrease in the fraction of sp3 bonds down to 20% because of the formation of nanocomposite structure in the form of graphite phase as sp2 clusters with size near 1.5 nm. An increase in the amplitude leads to the exponential decrease of the hardness and Young's modulus of the coatings down to 16 GPa and 166 GPa, respectively, and an increase in their plasticity.

The amplitude of the pulse in the range of 0.5-1 kV leads to the coatings being sufficiently hard (19-27 GPa) and having excellent adhesion to the steel substrate, at the level of HF-1 – HF 2. A combination of the high quality of the surface and a relatively small amount of microparticles makes such diamond-like carbon nanocomposite coatings useful for applications that require thick functional coatings.

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The Development of Nanostructuring Method Metal Surfaces by Electrospark Alloying

Oksana Gaponova[1*], Viacheslav Tarelnyk[2], Stanislav Marchenko[1], Ievgen Konoplianchenko[2], Nataliia Tarelnyk[2]

[1] *Sumy State University (Ukraine)*
[2] *Sumy National Agrarian University (Ukraine)*

* gaponova@pmtkm.sumdu.edu.ua

Abstract ID #MTFC-0716

The paper analyzes the works dedicated to solving surface nanostructuring methods. There are traditional technologies of nanostructured coating of chemical vapour deposition chemical (CVD) and physical vapor deposition (PVD) [1-3]. A new method is proposed, based on the use of concentrated flows of energy and matter, on electrospark alloying method (ESA) [4]. In [5] the author established that the ESA method allows controlling the dispersion of the crystalline structure of coatings. Nanostructuring of coatings can also occur due to the use of nanocomponents anodic materials. A method of obtaining nanostructured coatings by the ESA method with the use of special technological media (STM) created between the anode and the cathode (detail) and containing nanocrystalline particles in a dosed amount is proposed. There have been considered the features of the coating structure formation in the course of the ESA processing the Aarmco iron by the molybdenum electrode with the use of the STM composition with carbon nanotubes. The influence on the ESA regimes and the composition of the STM on the microstructure and hardness of the coatings has been considered. The microstructures after the ESA process consist of three zones: the upper "white" layer, which is not etched in the reagent, the diffusion zone and the base of a ferrite structure corresponding to the Armco iron. In the course of processing the Armco iron, with an increase in the discharge energy, the thickness and the continuity of the coating increases. In the microstructures, the nanoscale phases of 40 to 60 nm are detected, and they are evenly distributed in the coatings. Adding nanotubes provides an increase in hardness from 446 HV to 608 HV. Because of the ESA process, the coatings with a uniform distribution of molybdenum are formed. Carbon, apparently in the form of the carbon nanotubes, is concentrated on the surfaces of the samples being processed, regardless of the discharge energy during the ESA process. Their introduction to the STM helps to increase hardness and continuity. The addition of nanotubes has a positive effect on the quality of coatings.

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Epitaxial RTP Thin Films: The Rb^+ Diffusion Problem

Mathieu Salaün*, Benoit Boulanger
Université Grenoble Alpes (France)

* mathieu.salaun@neel.cnrs.fr

Abstract ID #MTFC-0728

The mm2 orthorhombic potassium titanyl phosphate crystal, i.e. $KTiOPO_4$ (KTP), is a famous biaxial nonlinear optical crystal widely used commercially for second harmonic generation (SHG) or optical parametric oscillation (OPO) pumped by a 1.064 µm Nd:YAG laser for example. Most of its applications are based on bulk single KTP crystals. However, there is a strong interest to elaborate submicrometric waveguides in the framework of integrated photonic devices. Among several waveguide-fabrication techniques such as proton exchange, ion implantation or dicing [1], a serious alternative is Pulsed Laser Deposition (PLD). Indeed, it was reported that type-II second-harmonic generation and sum-frequency mixing could be realized in uniform epitaxial $RbTiOPO_4$ (RTP) films over KTP channel waveguides prepared by PLD [2]. Such waveguides could be a serious alternative to efficient low energy nonlinear optical devices in particular for Telecom or spectroscopic applications.

PLD is a technique particularly well suited for growing single oxides films with complex chemical composition. This technique consists in a high energy laser ablation of a material with the same chemical composition than that of the desired layer. The plasma of the ablated material is then condensed on the substrate and heated to a temperature such as the aggregates can self-organise on the atomic lattice of the substrate leading to the epitaxial layer.

In this study, we performed epitaxial growth of the RTP phase on KTP single crystals by PLD. The target that has been used was a single RTP crystal. However, by chemical analysis and Xray diffraction we demonstrated that due to alkali interdiffusion between film and substrate, it was not possible to achieve a pure epitaxial layer of RTP but most likely an mixed stoichiometry $KxRb(1-x)TiOPO_4$.

More recently, we proposed to grow a very thin intermediate layer between substrate and RTP to avoid any diffusion. The material which has been chosen is cobalt orthosilicate (Co2SiO4). Indeed, this orthorhombic crystal has 2 cells parameters very closed to the RTP and KTP cells resulting in a lattice mismatch sufficiently low to allow an epitaxial growth.

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Tribological Properties of Few-Layer $Ti_3C_2O_x$ MXenes

Milan Tapajna*, Andrii Kozak
Centre For Advanced Materials Application CEMEA, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava (Slovakia)
* milan.tapajna@savba.sk

Abstract ID #MTFC-0740

Two-dimensional (2D) materials with a thickness of several atomic layers while extending in the other two dimensions exhibit outstanding friction effects such as superlubricity, stick-slip, puckering, friction hysteresis, or directional anisotropy [1]. Recently, a new class of 2D materials, referred to as MXenes, gained great attention in tribology research due to their excellent physical and chemical properties, good anti-corrosion properties, low friction, and high wear resistance. Thanks to its unique structure and ability to control the surface termination groups, MXenes represent extremely promising materials for solid lubrication applications. Up to now, mostly tribological properties of 2D MXenes as additive components in the solvents have been investigated [2], while very little is known about nanotribological properties of few-layer MXenes. We will present our recent results on the nanotribological properties of mono-, and double-layer Ti_3C_2Tx MXenes deposited by Langmuir-Schaefer technique on SiO_2/Si substrates [3]. Friction force of the monolayers was found to be slightly higher as compared to double and three-layer flakes, while double and three-layer flakes exhibit similar friction. This behavior is different from that typically observed for other 2D materials such as graphene, where friction force increases with number of layers due to the puckering effect. This behavior was explained by unique dominant mechanism of friction for $Ti_3C_2T_x$ MXenes, being identified as viscous regime at relatively high scanning velocities and the meniscus forces affected by contamination of the MXenes surface was proposed to control the friction at low sliding velocities.

Further, coefficient-of-friction (COF) of $Ti_3C_2T_x$ MXenes deposited on various steel substrates using spin-coating with and without TiO_2 interlayer were analyzed using standard ball-on-disc test. Samples were measured at different sliding parameters (applied load) and under different environment (vacuum and ambient air). Our results suggest that the use of softer substrates leads to less rigid contact, resulting in a possible transition of the tribo-layer from the coated substrate to the sliding counterparts and a reduction in friction. This effect can be observed in both air and vacuum in a long-term test. The hard TiO_2 interlayer in air results in abrasive wear of the coating as well as the steel substrates due to surface oxidation, which increases friction. In vacuum sliding, oxidation is reduced, however, friction forces increased due to the formation of a tribo-layer with a large number of defects and hard nanoparticles. All experiments illustrate excellent potential of $Ti_3C_2T_x$ MXenes for dry lubrication of open interfaces in both, air as well as vacuum ambient.

ACKNOWLEDGMENTS

This work was performed during the implementation of the project Building-up Centre for advanced materials application SAS, ITMS project code 313021T081 supported by Research & Innovation Operational Programme funded by the ERDF (50%) and Research and Development Agency under the contracts Nos. APVV-17-0560 and APVV-21-0231.

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Mechanical and Tribological Properties of Silver-Doped CrB_2 Thin Films Prepared by DC/Hipims Technology

Martin Truchlý[1] *, Marián Haršáni[2], Adam Frkáň[2], Tomáš Fiantok[1], Martin Sahul[3], Tomáš Roch[4], Peter Kúš[1], Marián Mikula[1]

[1] *Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava (Slovakia)*
[2] *Staton, s.r.o. (Slovakia)*
[3] *Faculty of Materials Science and Technology, Slovak University of Technology in Bratislava (Slovakia)*
[4] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*
* martin.truchly@fmph.uniba.sk

Abstract ID #MTFC-0759

The properties of transition metal diborides (TMBs), including their high melting temperature, chemical and thermal stability, high electrical and thermal conductivity, and high hardness level, have attracted a lot of attention in recent years [1]. Among them, chromium diboride (CrB_2) has received less attention, but nevertheless has some promising properties. In bulk form, it possesses a melting temperature of 2200 °C, a high bulk modulus (211 GPa), oxidation resistance up to 1000 °C, a low thermal expansion coefficient, good wear resistance, and chemical inertness [2]. Compared to titanium diboride (TiB_2), CrB_2 has better corrosion resistance [3]. Thus, CrB_2 is a viable candidate for various high-temperature applications.

Doping of TMB thin films with soft metal can extend their potential application in tribology and biomedicine. To prepare silver-doped CrB_2+x thin films on unheated substrates, a combination of direct current unbalanced magnetron sputtering and high-power pulsed magnetron sputtering (HiPIMS) was used. All thin films were over-stoichiometric, with a B/Cr ratio ranging from 2.05 to 2.30 and silver content varying from 3 at.% to 29 at.%. While thin films with lower silver content are X-ray amorphous, films with higher silver content have a nanocomposite structure containing silver grains embedded in an amorphous CrB_x matrix.

The reference $CrB_{2.3}$ thin film has the highest hardness of 26.6 GPa and an elastic modulus of 362 GPa. The addition of silver leads to a decrease in the hardness of Ag-CrB_{2+x} from 22.1 GPa to 7.8 GPa, accompanied by a decrease in the elastic modulus from 325 GPa to 187 GPa. The reference Ag thin film exhibits a hardness of 1.2 GPa and an elastic modulus of 97 GPa. Despite the low deposition temperatures, thin films have sufficient adhesion on WC-Co substrates, and the critical load is over 35 N. Doping CrB_{2+x} with silver significantly improved the frictional properties when the coefficient of friction against bearing steel decreased from 0.71 to 0.29. Additionally, an improvement in the wear rate of the films is observed because of the formation of a lubricating metal film.

The studied silver-doped over-stoichiometric Ag-CrB_{2+x} film appears to be a promising candidate for tribological applications where moderate hardness combined with a low coefficient of friction is required. Moreover, the ceramic composite containing silver particles can find application in the field of biomechanics.

ACKNOWLEDGMENTS

This work was supported by Scientific Grant Agency (Grant No. VEGA 1/0296/22). It is also the result of support under the Operational Program Integrated Infrastructure for the project: Advancing University Capacity and Competence in Research, Develop-ment and Innovation (ACCORD), co-financed by the European Regional Development Fund.

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Structure, Mechanical and Tribological Properties of Co-Sputtered Zr-Ag-B_2 Thin Films

Tomáš Fiantok[1*], Martin Truchlý[1], Viktor Šroba[1], Tomáš Roch[2], Vitalii Izai[1], Marek Vidiš[2], Marián Haršáni[3], Leonid Satrapinskyy[4], Marián Mikula[1]

[1] *Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava (Slovakia)*
[2] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*
[3] *Staton, s.r.o. (Slovakia)*
[4] *Comenius University in Bratislava (Slovakia)*

** tomas.fiantok@fmph.uniba.sk*

Abstract ID #MTFC-0762

ZrB_2 is representing an ultra-high temperature ceramic material with the potential to fulfill the stringent requirements of today´s industry. It possess an outstanding temperature stability, high hardness and excellent chemical inertness. However, potential of ZrB_2 in form of thin film is still limited by an intrinsic brittleness and poor tribological properties. Here, the combination of theoretical and experimental approach is used to investigate the effect of silver alloying on the stability, mechanical and tribological properties of hexagonal ZrB_2 thin films.

Calculations, using density functional theory, show that Ag atoms are strongly insoluble in the ZrB_2 and alloying itself has a considerable impact on its mechanical properties. Addition of silver leads to an improvement in ductility and tribological properties but at the cost of decrease in hardness. The experiments supported high insolubility of silver predicted by theory, where the magnetron co-sputtered $Zr_{1-x}Ag_xB_{2+\Delta}$ films form a segregated nanostructure consisting of separated hexagonal ZrB2 and cubic Ag phase. With increased Ag content, values of Young´s modulus drop from $EZrB_{2.31}$ = 375 GPa to value of $EZr_{0.26}Ag_{0.74}B_{0.89}$ = 154 GPa followed by decrease of hardness from $HZrB_{2.31}$ = 30 GPa to value of $HZr_{0.26}Ag_{0.74}B_{0.89}$ = 4 GPa. Material flow around the cube corner indents also demonstrates and supports the suppression of fracture development and indicates improved ductility. Improvement of tribological properties was also confirmed when coefficient of friction (COF) was reduced from $COFZrB_{2.31}$ ~ 0.9 to a value of $COFZr_{0.26}Ag_{0.74}B_{0.89}$ ~ 0.25 for all counterpart materials – steel ($100Cr_6$), Si_3N_4 and WC/Co.

ACKNOWLEDGMENTS

This work was supported by Scientific Grant Agency (Grant No. VEGA 1/0296/22). It is also the result of support under the Operational Program Integrated Infrastructure for the project: Advancing University Capacity and Competence in Research, Develop-ment and Innovation (ACCORD), co-financed by the European Regional Development Fund. DFT simulations were carried out using the resources provided by the Swedish National Infrastructure for Computing (SNIC) and partially funded by the Swedish Research Council (Grant Agreement VR-2018-05973).

Corrosion Resistance of Tantalum-Based Coatings on Medical Implants

Stanislav Yakovin*, Stanislav Dudin, Alexander Zykov, Nina Yefimenko, Oleksandr Dakhov
V.N. Karazin Kharkiv National University (Ukraine)
* stanislav.yakovin@karazin.ua

Abstract ID # MTFC - 0766

Modern medicine widely uses implants and stents, which should ensure long-term operation in the patient's body, causing minimal harm. Various metals and compounds used to make implants and stents have the necessary mechanical properties, but the presence of metal in the human body can lead to undesirable consequences (increased exudation, formation of excess fibrosis, rejection reaction).

o solve this problem, thin-film coatings are widely studied for medical devices based on oxides and nitrides of transition group metals. Coatings of tantalum (Ta), tantalum nitride (TaN), tantalum oxynitride (TaON), and tantalum oxide (Ta2O5) demonstrate high corrosion resistance and characteristic biocompatibility. Currently, it is necessary to justify the use of tantalum-based coating materials for use in surgical practice.

This paper reports the results of a comparative experimental study of corrosion resistance of Ta-based bioinert coatings on metal samples. The idea of the research is to find the optimal coating for medical implants balancing corrosion resistance of oxides, high hardness of nitrides and ductility of metals. Biochemical and morphological substantiation of the use of tantalum-based coatings in surgical practice will be carried out at the following step of research through in vivo experiments using laboratory animals. Here we present the results of the corrosion resistance estimation of different Ta-based coatings studied using potentiostatic measurements.

Polished plates of medical stainless steel (AISI 304) measuring (1.5x1.5) cm and 2 mm thick were made for the application of Ta-based coatings. Such model implants are planned to be used for implantation in laboratory animals in the future. Various implants were coated with Ta, Ta2O5, TaN, and TaON (thickness of about 2 μm) by reactive magnetron sputtering using the multifunctional Cluster Ion-Plasma System (CIPS) [1-2], which consists of compatible sources of fluxes of metal atoms, ions, chemically active particles for a complex effect on the growing film.

Subsequently, coated and uncoated implants were tested for corrosion resistance. Polarization curves were measured in saline solution. The measurement results show that the tantalum oxide exhibits excellent insulating properties, but this result is not stable. The reason for this is that tantalum oxide is hard and brittle and the corrosion current is mainly due to defects in the coating. Tantalum, being a ductile metal, has the fewest defects and shows the most stable results. In this case, the corrosion current is only slightly inferior to the values for the oxide. Tantalum nitride has the highest corrosion current, while oxynitride shows intermediate results.

Thus, from the results of the research presented in this paper, it can be concluded that tantalum-based coatings can become one of the most practical ways to improve the durability and stability of biomedical implants and reduce the risk of post-surgery complications.

ACKNOWLEDGMENTS

This research was supported by the National Research Foundation of Ukraine in the framework of the project 2021.01/0204

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Highly Transparent, Colorless Optical Film with Outstanding Mechanical Strength and Folding Reliability Using Mismatched Charge-transfer Complex Intensification

Sung Woo Hong*, In Park, Dohoon Lee
Korea Institute of Industrial Technology (KITECH) (Republic of Korea)
* swhong@kitech.re.kr

Abstract ID #MTFC-0782

The development of flexible, transparent, and colorless optical films with exceptional mechanical properties is of great interest for the advancement of flexible displays and electronics. In this study, we report the development of a novel optical film with outstanding mechanical strength and folding reliability by utilizing the concept of mismatched charge-transfer complex (CTC) intensification.

The newly produced optical film achieves a tensile modulus of over 10 GPa, total transmittance close to 90%, and a yellow index below 3.0, demonstrating the best-recorded balance between mechanical strength and optical properties for a highly flexible optical film, to the best of our knowledge. Additionally, it has a superior pencil hardness grade (2H) compared to commercially available optical-grade engineering plastic films, and it exhibits exceptional mechanical durability and folding reliability for over 300,000 folding/unfolding cycles at a radius of 1.5 mm, surpassing currently available optical-grade engineering plastic films and glass substrates. These remarkable properties are attributed to a unique supramolecular structure with multiple hydrogen bonding and salt complexation interactions, which exhibits CTC intensification. We also propose a mechanism to explain the concept of mismatched CTC intensification.

In summary, our study provides valuable insights into developing highly flexible films with excellent optical properties, mechanical bulk and surface strength, mechanical durability, and folding reliability for next-generation flexible displays and electronics. Our findings also offer new possibilities for the design of advanced flexible displays and electronics, with potential applications in various fields, such as wearable devices, biomedical sensors, and flexible solar cells.

ACKNOWLEDGMENTS

The authors acknowledge the financial support of the Ministry of Trade, Industry and Energy, Republic of Korea (20011253) and the National Research Council of Science & Technology (NST), Republic of Korea (CRC22031-000).

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Corrosion Resistance Enhancement of Porous Titanium by Thermo-Chemical Treatment

Serhii Lavrys[1*], Khrystyna Shliakhetka[2], Iryna Pohrelyuk[1]
[1] *Karpenko Physico-Mechanical Institute of the National Academy of Sciences of Ukraine (Ukraine)*
[2] *Centre for Advanced Materials Application SAS (Slovakia)*
* lavrys92@gmail.com

Abstract ID #MTFC-0783

Powder metallurgy is a potentially cost-effective alternative to the conventional manufacturing of titanium. This technology has the advantage of near-net-shape formation and the non-requirement of high processing temperatures above the alloy melting point compared to conventional manufacturing [1, 2]. It should be noted that titanium manufacturing by powder metallurgy has structural features – porosity. It should be noted that titanium manufacturing by powder metallurgy has structural features – porosity, which negatively affects its corrosion resistance. It limits using low-cost porous titanium instead of wrought one in the chemical industry [3, 4]. In these studies, it was proposed to improve the corrosion resistance of porous titanium (porosity ~ 7%) by thermo-chemical treatment (nitriding, oxidation, Carbooxidation, and carbonitriding). The corrosion resistance of surface-treated porous titanium was evaluated by the static immersion test according to ASTM Standard G31-72(2004) in 20 wt.% HCl and 40 wt.% H_2SO_4 solutions. The wrought titanium produced by conventional technology was also used as a benchmark for comparison. Carboxide and carbonitride coatings formed on porous titanium were found to be either ineffective (20% HCl) or provide very low protection (40% H_2SO_4), which was attributed to the formation of inhomogeneous surface protective films as a result of the poor interaction of surface pores with a multicomponent environment, containing gas and powder components. Instead, oxidation and nitriding reduce the corrosion rate of porous titanium by 2-3 orders compared to untreated ones. In addition, the corrosion resistance of surface-treated porous titanium is approximately the same as for surface-treated wrought titanium.

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Experimental Investigation on Structure and Mechanical Properties of WN_x/TiSiN Nanocomposite Multilayer Coatings

Martin Sahul[1*], Barbora Bočáková[2], Marián Haršáni[3], Kateryna Smyrnova[4], Martin Truchlý[5], Miroslav Sahul6, Martin Kusy[7], Lubomír Čaplovič[2], Alexander Pogrebnjak[4,7], Tomáš Vopát[8]

[1] *Faculty of Materials Science and Technology, Slovak University of Technology in Bratislava (Slovakia)*
[2] *Slovak University of Technology (Slovakia)*
[3] *Staton, s.r.o. (Slovakia)*
[4] *Sumy State University (Ukraine)*
[5] *Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava (Slovakia)*
[6] *Faculty of Mechanical Engineering, Czech Technical University in Prague (Czech Republic)*
[7] *Faculty of Material Science and Technology in Trnava, Slovak University of Technology in Bratislava, Trnava (Slovakia)*
[8] *Slovak University of Technology in Bratislava (Slovakia)*

* martin.sahul@stuba.sk

Abstract ID #MTFC-0807

Multilayer coatings that usually consist of two different alternating layers with varying individual layer thicknesses have been successfully used as protective materials in many tribological applications and cutting tool industry [1]. The main advantage of the multilayer design is the possibility to achieve qualitatively new properties by combining two different materials. Monolithic tungsten nitride (WN) possesses high hardness, melting point, electrical conductivity, and chemical stability. Despite the excellent wear-resistant properties of this coating, only a few WN based multilayers in combination with the second transition metal nitride layer (WN/TiAlN [2], WN/CrAlSiN [3], WN/NbN [4]) have been prepared and studied so far. Ti-Si-N coating is characterized by a low friction coefficient, oxidation resistance, and thermal stability. The structure of the coating consists of nanocrystalline TiN grains surrounded by Si3N4 matrix, which makes it the best candidate in cutting of difficult-to-cut materials [5]. Thus, WN and Ti-Si-N based multilayer is expected to have enhanced wear and mechanical properties.

In the present study, investigations on the structure, phase composition and mechanical properties of a novel type of transition metal nitride-based coatings, namely WNx/TiSiN nanocomposite multilayers, are presented. The multilayers were deposited on tungsten carbide (WC/Co) substrates by magnetron sputtering from W (purity 99.95 %) and $Ti_{80}Si_{20}$ (purity 99.5 %) targets. During the depositions, the deposition time of individual WNx and TiSiN layers increased from 20 s to 120 s, which resulted in a change in the multilayer bilayer period. The effect of the bilayer period on the structure, phase composition and mechanical properties represented by hardness and elastic modulus of WNx/TiSiN multilayers was comprehensively studied by scanning electron microscopy (SEM), wave dispersive X-ray spectroscopy (WDS), grazing incidence X-ray diffraction (GI-XRD) and nanoindentation (NI).

The bilayer periods (Λ) increased from 28.8 ± 1.2 nm to 172.8 ± 12.3 nm with increasing deposition time from 20 s to 120 s. The GI-XRD revealed that all multilayers had polycrystalline structures with similar phase compositions. WNx layer consisted of the body-centered cubic (BCC) W phase and TiSiN layer exhibited the face-centered cubic (FCC) TiN phase. The highest hardness of 32.7 ± 2.1 GPa was documented in the case of multilayer with the bilayer period of 57.6 ± 2.2 nm (multilayer deposited with deposition time of 40 s for every layer). The multilayer also exhibited the highest H/E and H3/E2 ratios of 0.088 and 0.254, respectively, indicating improved fracture toughness and resistance to deformation. However, the highest elastic modulus of 380.6 ± 24.1 GPa was observed at the bilayer period of 172.8 ± 12.3 nm (deposition time of 120 s). It can be concluded that the WNx/TiSiN multilayer is a promising candidate in the protection of cutting tools.

ACKNOWLEDGMENTS

This research was funded by the VEGA Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and Slovak Academy of Sciences, grant number 1/0345/22. It was also supported by the Erasmus+ ICM 2020 program, project code 2020-1-SK01-KA107-078196, and the Slovak Research and Development Agency (APVV) joint bilateral project Slovakia - Ukraine 2021, project number SK-UA-21-0032.

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Antimicrobial Ag Nanoclusters in Hard TiB_2 Matrix Prepared by Magnetron Sputtering

Marek Vidiš[1*], Martin Truchlý[2], Vitalii Izai[2], Tomáš Fiantok[2], Miroslav Rajninec[3], Tomáš Roch[1], Leonid Satrapinskyy[4], Stefan Nagy[5], Veronika Turiničová[1], Marián Mikula[2]

[1] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*
[2] *Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava (Slovakia)*
[3] *Institute of Plant Genetics and Biotechnology, Slovak Academy of Sciences (Slovakia)*
[4] *Comenius University in Bratislava (Slovakia)*
[5] *Institute of Materials and Machine Mechanics, Slovak Academy of Sciences (Slovakia)*
*marek.vidis@fmph.uniba.sk

Abstract ID #MTFC-0808

Due to strong antimicrobial properties, silver nanoparticles are often used to functionalize materials. Considering the threat of developing Ag resistant bacteria [1], it is important to address the endurance of such materials and to control the amount of Ag released into the environment [2]. The release rate can be moderated by creating a nanocomposite of Ag embedded in a wear-resistant matrix that protects the Ag from premature depletion [3]. In this work, we used conventional magnetron co-sputtering to prepare Ag nanoclusters embedded in the hard titanium diboride thin film. The Ag does not dissolve in TiB_2, as implied by the positive formation energy of AgB2 obtained by DFT calculations [4]. Therefore, instead of the $Ag_xTi_{1-x}B_2$ solid solution, a formation of segregated Ag clusters can be expected. This is confirmed by the transmission electron microscopy that reveals spherical-like Ag nanoclusters with sizes of 2–3 nm for Ag/TiB_2 film with 1.4 at.% Ag. The antibacterial effect increases with the Ag concentration and the strongest growth inhibition of 97%, compared to the uncoated substrate, is reached for film with 24 at.% Ag. The segregated Ag slowly releases into the environment, as confirmed by the measurement of Ag concentration in the solution for the as-deposited samples and for samples immersed for 45 days. Alloying with silver also results in a decrease in hardness from 40 GPa for pure TiB2+x to 7.9 GPa for film containing 24 at.% Ag. The hardness drop can be explained by the suppression of the columnar growth of TiB2 in the (001) direction as well as by the introduction of a much softer Ag phase localized between the TiB_2 grains. On the other hand, silver has a positive impact on the tribological properties, decreasing the friction coefficient from 0.77 to 0.35, and on the specific wear rate which reaches low values of 2.2–6.4 × 10-5 mm3/Nm despite the observed hardness decrease.

ACKNOWLEDGMENTS

This research was funded by Operational Program Integrated Infrastructure (Project No. ITMS 313011AUH4) and by Scientific Grant Agency (Grant No. VEGA 1/0296/22).

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The Concept of Improving Mechanical Properties and Fracture Toughness in Multilayered Coatings Based on Transition Metal Diborides

Marian Mikula[1*], Marek Vidiš[1], Marek Gocník[1], Tomáš Fiantok[2], Viktor Šroba[2], Vitalii Izai[2], Martin Truchlý[2], Leonid Satrapinskyy[3], Stefan Nagy[4], Branislav Grančič[1], Peter Kúš[2]
[1] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*
[2] *Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava (Slovakia)*
[3] *Comenius University in Bratislava (Slovakia)*
[4] *Institute of Materials and Machine Mechanics, Slovak Academy of Sciences (Slovakia)*
*mikula@fmph.uniba.sk

Abstract ID # MTFC- 0811

Diborides of transition metals belong to the group of ultra-high-temperature ceramics and have a high application potential in the form of bulk material as well as coatings in the machining and aircraft industries. Current experimental research is focused on the physical preparation of monolithic diboride coatings based on elements of the IVB, VB and VIB groups (Ti, Zr, Cr, Ta, Nb, Mo, W). The resulting coating structure often has a nanocomposite character formed by nanocrystalline filaments covered by an amorphous tissue phase and exhibits extreme hardness values of around 40 GPa. Unfortunately, these excellent mechanical properties are accompanied by typical problems of these ceramic materials – affinity to crack formation and weak plastic response against deformation. Research on similar types of coatings based on transition metal nitrides indicated that a promising way to suppress the formation and propagation of cracks is the periodic alternation of chemically or structurally different nitrides with a thickness of several nanometers, the so-called superlattices (SL) or multilayers (ML). This concept is transferred to the field of diboride coatings in the presented lecture. Here, we investigate TiB_2/TaB_2 coatings prepared by magnetron sputtering from two stoichiometric targets where the thickness of individual layers, the so-called bi-period l vary between 4÷12 nm (SL) and 20÷40 nm (ML). These differences in the thicknesses of individual layers lead to the formation of a different structure and show different mechanical and fracture-mechanical behavior compared to the basic binary constituents. Understanding these differences requires several non-trivial experimental approaches involving demanding analytical investigations at the nanoscale level, e.g., using transmission electron microscopy and a series of measurements of fracture-mechanical properties of selected TiB_2/TaB_2 coatings using cantilevers bending tests - to determine stress intensity factor K_{IC}.

ACKNOWLEDGMENTS

This work is supported by the Slovak Research and Development Agency [Grant No. APVV-21-0042] and European Space Agency (ESA Contract No.4000136772/21/NL/SC/hm) and the Operational Program Integrated Infrastructure for the project: Advancing University Capacity and Competence in Research, Development, and Innovation (ACCORD), co-financed by the European Regional Development Fund. M.M. thanks to Dr. Michael Meindlhumer from Erich Schmid Institute in Leoben, Austria for cantilevers bending tests.

Study of Thermomechanical Properties of Multilayer Nanocomposite Film Systems

Oleksandr Goncharov[1,2*], Alexei Khomenko[1], Anna Badalian[1], Dmitry Belous[1]
[1] *Sumy State University (Ukraine)*
[2] *Institute of Materials Science, Slovak University of Technology in Bratislava, Trnava (Slovakia)*
* o.goncharov@mss.sumdu.edu.ua

Abstract ID #MTFC-0812

The application of nanocomposite nanostructured coatings on the surface of the contacting work zones, which are under the influence of significant thermal or physical and chemical loads, protects the surface and increases its operational characteristics [1, 2]. In our works, a study of the influence of carbide and nitride film systems on thermal and deformation processes in solution zones with different compositions of the corresponding structures was carried out [3, 4].

The paper presents modeling and research of the state of thermal and deformation fields for a plate made of AISI/SAE 1045 steel without coating, with a single-layer coating of TiN, with a double-layer coating of TiCN/α-Al2O3 and a coating of TiN/α-Al2O3, and with a three-layer coating of TiN/α- Al2O3/TiCN. The processes of heat transfer and the peculiarities of the formation of strain-stress fields in the cutting tool depending on the structural composition and the state of multilayer film coatings were investigated. The effect of a nano-sized multilayer film system of different composition on the spread of thermal and strain-stress fields in the cutting zone under the influence of thermal load was investigated. It was established that the magnitude and law of distribution of mechanical stresses, deformation processes in multicomponent systems are determined by the nature of the temperature field.

A mathematical model is presented that describes the deformation processes in the surface layers of the cutting surface by a system of differential equations based on the synergistic Lorentz system with the order parameters of deformation and stress. The results of the study in the form of constructed phase portraits of the system showed special points that allowed us to draw conclusions about the influence of the coating on the stress-strain characteristics of the surface structure of the material. The evolution of the system was studied.

The thermal and mechanical characteristics of nanocomposite multilayer coatings are compared depending on their structural and phase state. The processes of heat transfer and the formation of strain-stress fields in the cutting tool are analyzed depending on the structural state and, accordingly, the physical and mechanical characteristics of multilayer film coatings.

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Sputtering as a Versatile Technique for the Production of Nanomaterials for Diverse Applications

Albano Cavaleiro[1,2*]
[1] *University of Coimbra (Portugal)*
[2] *Instituto Pedro Nunes, Coimbra (Portugal)*
* albano.cavaleiro@dem.uc.pt

Abstract ID # MTFC-0821

Sputtering is a bottom up processing technique based on the sequential deposition of individual atoms/molecules onto a substrate to produce a thin film or a coating. By playing with the composition of either the materials sources (targets) or the gases environment as well as the deposition conditions, different structural and morphological arrangements can be produced in the thin films. Monolithic, graded and multilayer cross section morphologies can be easily deposited allowing to achieve specific properties required for particular applications. Epitaxial, nanocrystalline, nanocomposite or amorphous structures can be controlled and varied in the same system of chemical elements.

In this talk, several examples of sputtered films will be presented showing the potentiality of sputtering for tailoring the morphology and/or the structure of thin coatings to fulfil the objectives required for specific applications. These examples were selected based on cases inspired on either the nature or old empirical human knowledge, to develop high performing coatings regarding mechanical and optical properties. The procedure and processing steps behind the tailoring of a coating as a function of the required properties will be also presented and discussed.

High Entropy Alloy Composite Coating Material and Its Application

Bing Yang*
School of Power Mechanical Engineering, Wuhan University, Wuhan, 430072 (China)
*yangbing@whu.edu.cn

Abstract ID # MTFC-0823

High entropy alloys which are usually composed of at least five primary elements exhibit better performance than the conventional alloys in terms of high hardness, high toughness and high-temperature resistance, based on their unique high entropy effect, lattice distortion effect, sluggish diffusion effect and cocktail effect, thus showing great potential for application in the field of protective coatings. However, the research on high-entropy alloy coatings is still in its initial stage, and there is a lack of in-depth research on the structure and performance of the coatings. In this paper, the high entropy metallic, nitride, nitrogen oxide and oxide coatings based on AlCrNbSiTi were fabricated using magnetron sputtering and arc ion plating techniques. The evolution of the phase composition, grain scale, orientation and other microstructures of the coatings were characterized, and the mechanical properties, friction behaviour, temperature resistance and corrosion resistance of these coatings were investigated systematically. The toughness mechanism and elemental coupling were explored. The wear friction behaviour and the elemental diffusion law and the oxidation mechanism of the coatings at high temperatures were studied. The electrochemical corrosion behaviour of the coatings was investigated as well. Finally, according to the actual engineering needs, the application prospect of high entropy coating in die casting dies, tools and parts is discussed.

Analysis of the Mechanical Properties of WN_X/TiSiN Nanocomposite Multilayer Coating and Its Monolithic WN_X and TiSiN Layers

Martin Sahul[1], Barbora Bočáková[2*], Marián Haršáni[3], Kateryna Smyrnova[4], Miroslav Sahul[5], Martin Truchlý[6], Martin Kusy[7], Lubomír Čaplovič[2]

[1] *Faculty of Materials Science and Technology, Slovak University of Technology in Bratislava (Slovakia)*
[2] *Slovak University of Technology (Slovakia)*
[3] *Staton, s.r.o. (Slovakia)*
[4] *Sumy State University (Ukraine)*
[5] *Faculty of Mechanical Engineering, Czech Technical University in Prague (Czech Republic)*
[6] *Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava (Slovakia)*
[7] *Faculty of Material Science and Technology in Trnava, Slovak University of Technology in Bratislava, Trnava (Slovakia)*

* barbora.bocakova@stuba.sk

Abstract ID #MTFC-0827

Transition metal nitride (TMN) based coatings have been widely utilized due to their high hardness, low coefficient of friction, good thermal stability, and oxidation resistance [1]. Therefore, hard nitride coatings are popular in machining industry for improving the lifetime of cutting tools [2]. One of the most industrially used coatings is the TiSiN coating, which excellent anti-wear properties are attributed to the nanocomposite structure that consists of nanocrystalline TiN grains embedded in amorphous silicon nitride matrix [3]. It is well known that the tribo-mechanical characteristics of the TiSiN coating strongly depend on microstructure and Si content [4]. However, the methods for enhancement of the properties of these coatings are currently strongly limited. Therefore, one of the affordable possibilities to further improve the properties of coatings is the use of a multilayer design. The multilayer architecture significantly improves the adhesion, toughness, and anti-wear properties of the coatings. Tungsten nitride (WN) was chosen as the second layer because of the convenient combination of excellent hardness, high melting point, good chemical stability, and high conductivity [5].

In the current paper, WN_x/TiSiN nanocomposite multilayer and its WN_x and TiSiN monolithic coatings have been fabricated by unbalanced direct magnetron sputtering using the same deposition parameters. All coatings were deposited on high-speed steel (HSS) discs employing W (purity 99.95 %) and $Ti_{80}Si_{20}$ (purity 99.5 %) targets. The aim was to study the effect of the multilayer design on the structure, phase composition and mechanical properties (hardness, elastic modulus, H/E and H^3/E^2 ratios) of the WN_x/TiSiN multilayer. The microstructure and chemical composition of coatings were studied by scanning electron microscopy (SEM) and wave dispersive X-ray spectroscopy (WDS). X-ray diffraction (XRD) was performed for the analysis of the structure. Furthermore, mechanical properties were analysed by the nanoindentation testing (NI).

It has been proved that the WN_x/TiSiN multilayer consisted of cubic W and TiN phases. The microstructure of the multilayer was dense with no defects at interfaces of individual layers. Compared to the WNx and TiSiN monolithic coatings, the multilayer showed slightly improved hardness (28.5 ± 3.5 GPa) and H/E parameter (0.087). Based on above, the multilayer design of the WN_x/TiSiN coating is a promising way to enhance the microstructure and mechanical properties of the hard coatings.

ACKNOWLEDGEMENTS

This research was funded by the VEGA Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and Slovak Academy of Sciences, grant number 1/0345/22. It was also supported by the Erasmus+ ICM 2020 program, project code 2020-1-SK01-KA107-078196, and the Slovak Research and Development Agency (APVV) joint bilateral project Slovakia - Ukraine 2021, project number SK-UA-21-0032.

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High-Entropy Diboride Films: Experimental and First-principles Investigations

Volodymyr Ivashchenko[1,2*], Petro Scrynskyy[1], Aleksey Onoprienko[1], Alexander Pogrebnjak[3,2], Andrii Kozak[1,4], O. K. Sinelnichenko[1], D. V. Vedel[1], Pavlo V. Mazur[1]

[1] *Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, Kyiv (Ukraine)*

[2] *Faculty of Material Science and Technology in Trnava, Slovak University of Technology in Bratislava, Trnava (Slovakia)*

[3] *Sumy State University (Ukraine)*

[4] *Centre for Advanced Materials Application, Slovak Academy of Sciences, Bratislava (Slovakia)*

* volodymyr.ivashchenko@gmail.com

Abstract ID #MTFC-0834

DC magnetron sputtering of a target composed of TiB_2, ZrB_2, HfB_2, NbB_2 and TaB_2 was applied to prepare high-entropy (Ti, Zr, Hf, Nb, Ta)B_2 solid solution thin films. The films were deposited at various substrate biases (from 0 to -250 V) and were investigated with XRD, AFM, XPS, Raman spectroscopy, indentation and tribological tests. The XRD and XPS studies indicate that the films consist of the single-phase crystallites of the solid solutions based on the constituent diborides with the preferable orientation (001). The film with a grain size of about 20 nm has the high hardness of 38 GPa, however, lower than that of the TiB 2 films (51.5 GPa). The dependence of hardness on the substrate bias is the result of competitive of the Hall-Petch effect and compressive stress due to ion bombardment of growing film. The highly biased film that possesses the lowest hardness exhibits the smallest value of friction coefficient (0.49). The film surfaces are smoothing: their root mean square roughness does not exceed 0.37 nm.

The stability, electronic structures and mechanical properties of the random (TiZrHfMTa)B_2 diborides, M=Sc, V, Nb, Mo, (HED-Sc, HED-V, HED-Nb, HED-Mo alloys, respectively) and the constituting binary diborides was studied in the framework of a first- principles approach. The mixing energy of all the HEDs is negative, excepting HED-V. This high entropy diboride is unstable against the decomposition into the constituent diborides. The highest hardness is found to be reached for the HEDs with an valence electron concentration equal to 10, as in TiB_2 . It was shown that the mechanical characteristics (shear and Young moduli, Vickers hardness, fracture toughness, Debye temperature) of the quinary diborides based on TiB_2 are not higher than those of TiB_2 and are close to the average values of the corresponding characteristics of the constituting diborides. The experimental and theoretical results obtained in this investigation are discussed in comparison with those of other authors on high-entropy diboride films and bulk materials.

Integrity of Graphene or Nanoparticles in Functional Nanostructures Represented by Resistively Switching Media Grown by Atomic Layer Deposition

Aile Tamm*
University of Tartu (Estonia)

* aile.tamm@ut.ee

Abstract ID #MTFC-0845

Dramatic growth of information density and data related to the development of artificial intelligence (AI) necessitates increment in computing performance. Neuromorphic computing could, in addition, decrease the power consumption [1]. Electronic switches, also characterized by rather simple structure, are searched upon research and development of next-generation nonvolatile resistive random-access memory (RRAM) prototypes. Artificial mixing of different oxides and graphene as interface layer order to tailor their useful physical properties could allow the extension of their application areas including potential memory materials [2].

Metal nanoparticles of chemical vapor deposited graphene can be transferred to Si/SiO2 or Si/TiN substrates or different metal oxide films. Thin layers of metal oxides, such as Al_2O_3, HfO_2, ZrO_2 or Ta_2O_5 can then be grown by plasma-assisted atomic layer deposition (ALD) on transferred graphene or layer of nanoparticles. Nanostructures containing graphene/nanoparticles were, thus, synthesized and analysed, keeping in mind their potential applications in nanoelectronics (RRAM), and also nanosensors, electrodes for energy storage and harvesting devices.

The metal oxide films have been deposited either in a commercial PicosunTM R-200 Advanced ALD system or in low-pressure flow-type home-build reactors. Graphene sheets were grown on commercial 25 μm thick polycrystalline copper foils in an in-house built chemical vapour deposition (CVD) reactor, and transferred onto Si/SiO_2 or Si/TiN or Si/TiN/metal oxide substrates by using a wet chemical transferring process described by Kahro et al. [3]. Thereafter, metal oxide layers could be grown on top of graphene in plasma-assisted processes without destruction of its integrity.

Stacked nanostructures with nanoparticle or graphene layer intermediating metal oxide insulators, devised as resistive switching media between top Ti, or Au, and bottom TiN electrodes, were studied comparatively with and without graphene/nanoparticles interlayers. The switching processes could, apparently, be promoted in the devices supplied with conductive interlayer, compared with the media consisting of insulating dielectric oxide films only.

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A Comparative Study of Microstructure and Properties of TiZrN/NbN and TiSiN/NbN Nanolaminate Coatings

Olga Maksakova[1,2*], Vyacheslav Beresnev[2], Sergiy Lytovchenko[2], Diana Kaynts[3]
[1] *Faculty of Materials Science and Technology, Institute of Materials Science, Slovak University of Technology in Bratislava, 25, Jána Bottu Str., 917 24 Trnava (Slovakia)*
[2] *V.N. Karazin Kharkiv National University, 4, Svoboby Sq., 61000 Kharkiv (Ukraine)*
[3] *Uzhhorod National University, Uzhhorod (Ukraine)*
* maksakova.tereshenko@gmail.com

Abstract ID # MTFC-0854

As a superhard coating material, multilayer nanolaminates are one of the hot points in recent decades [1-3]. In nanolaminates, the downscaling of the multilayer architecture to the nanometric regime allows for further extending the functional benefits of coatings through the expression of synergistic properties arising from the small-scale heterogeneity of the coating, such as the establishment of stress gradients impeding dislocations and cracks propagation, a phenomenon often referred to as the superlattice-effect. Due to these distinctive phenomena, these materials are becoming popular in diverse applications that require high strength, increased ductility and fracture toughness, wear and oxidation resistance, shock resistance, biocompatibility, and certain optical properties. To our best knowledge, no report exists on the development and experimental analysis of TiZrN/NbN and TiSiN/NbN nanolaminates. In the attempt to fill this vacancy, here we report on the compare the microstructure and mechanical properties of cathodic-arc deposited TiZrN/NbN and TiSiN/NbN nanolaminates. We found that in the case of TiSiN/NbN nanolaminate the crystallographic structure of the modulation layer consisted of fcc-TiN+a-SiNx in TiSiN nanolayer and fcc-NbN+hcp-NbN-δ' in NbN nanolayer multiphases. The crystallographic structure of TiZrN/NbN nanolaminate was also multiphase: fcc-TiN+fcc-ZrN in TiZrN nanolayer and fcc-NbN+hcp-NbN-δ' in NbN nanolayer. From the low-magnification image of TiSiN/NbN nanolaminate, it was clear that no columnar growth structure can be observed, suggesting that the insertion of TiSiN nanolayers destructed the columnar growth structure, which made its cross-sectional morphology featureless. From the high-magnification image, it could be seen that TiSiN nanolayers exhibit an amorphous state, implying that the "template effect" of NbN nanolayers on TiSiN nanolayers disappears. The amorphous TiSiN nanolayers blocked the epitaxial growth structure between NbN nanolayers. At the low-magnification image of TiZrN/NbN nanolaminate, it was obviously clear that the coating was a columnar growth structure, indicating that the insertion of TiZrN nanolayers could not prevent the columnar growth structure. In the high-magnification image, it was clear that the lattice fringes continuously went through several modulation nanolayers, indicating that TiZrN nanolayers had partially transformed into the crystalline structure under the "template effect" of NbN nanolayers and grown coherently with NbN nanolayers. The mechanical properties were the following: for TiZrN/NbN nanolaminate the hardness was 40.6 GPa and the elastic moduli was 597 GPa, and for TiSiN/NbN nanolaminate the hardness was 40 GPa and the elastic moduli was 560 GPa. The above results suggest that with different constituent elements, the multilayer TiZrN/NbN and TiSiN/NbN nanolaminates exhibit different morphologies, which lead to different microstructures and mechanical properties.

ACKNOWLEDGEMENTS

This research is supported by the Ukrainian state budget program No. 0122U001659.

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Graphene Oxide Modified by Fluoropolymer Brushes as a Promising Lubricant in Ambient Air and Vacuum

Andrii Kozak[1*], Markéta Ilčíková[2], Nafiseh Babaei[3], Nikolaos Konios[3], Marián Precner[4], Josef Osička[5], Jaroslav Mosnáček[2], Milan Tapajna[1]

[1] *Centre For Advanced Materials Application CEMEA, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava (Slovakia)*

[2] *Centre for Advanced Materials Application SAS, Dúbravská cesta 9, Bratislava 845 11, Slovakia (Slovakia)*

[3] *Polymer Institute SAV, Dúbravská cesta 9, Bratislava 845 41, Slovakia (Slovakia)*

[4] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*

[5] *Centre of Polymer Systems, Tomas Bata University, Trida Tomase Bati 5678, Zlin 76001, Czech republic (Czech Republic)*

* andrii.kozak@savba.sk

Abstract ID # MTFC-0882

Graphite retains one of the most commonly used lubricant for a long time, however, in a dry or vacuum environment its low friction performance is reduced due to the increase of the interlamellar binding energy [1]. Monolayered graphene can sufficiently reduce friction in vacuum conditions, however, the surface modification of the graphene is challenging. On the other hand, graphene oxide (GO) offers more controllable mechanical, electrical, and tribological properties. In this work, we investigated the impact of the modification of the GO layers by fluoropolymer brushes on the macroscale friction coefficient (COF) in both air and vacuum conditions.

GO layers were grafted with poly(trifluoroethyl methacrylate) brushes under surface initiated atom transfer radical polymerization conditions. The molar mass of brushes was 73,200 g/mol (GPC, PS calibration). After sintering of the mono and a few-layered powders, they were diluted in the DMF with a concentration of 50mg/mL, and spin-coated on the sapphire substrates. The ball-on-disc friction experiment has been performed in the relative oscillatory motion system by using Al_2O_3 and Si_3N_4 balls as a counterpart. Ambient air tribological investigations prove a good lubrication effect of all the coatings as compared to the sapphire substrate by the formation of a GO and reduced GO (rGO) tribofilm. However, PTFEMA-modified GO layers are characterized by three times lower friction as compared to pristine GO ones (0.6 and 0.2, respectively). This difference is supposed to be caused by the reduction and modification of the GO layers by PTFEMA brushes, which decreases the surface hydrophilicity and decreases the friction at the interface. Moreover, better separation of the PTFEMA-modified GO layers results in a lower number of wear debris formation, which facilitates the replacement of the defective GO agglomerations with rGO tribofilm, reducing the friction. In contrast, the tribofilm formed on the sliding ball surface resulted in a similar COF for all the coatings in vacuum. The COF in a vacuum is close to 0.11 and notably lower than one in the air, which is caused by saving the lamellar structure, and lowering debris agglomerations due to the absence of hydrogen bonds between GO lamellas caused by water vapours.

Obtained results demonstrate that modification of the GO layers by polymer brushes could sufficiently reduce the effect of the wear debris on the COF, which will increase the lifetime of applications working in extreme conditions.

ACKNOWLEDGEMENTS

This work was performed during the implementation of the project Building-up Centre for advanced materials application SAS, ITMS project code 313021T081 supported by Research & Innovation Operational Programme funded by the ERDF (50%) and Research and Development Agency under the contracts APVV-17-0560, APVV-21-0231 and APVV-19-0338. M.I. and J.O. acknowledge the Ministry of Education, Youth and Sports of the Czech Republic - DKRVO (RP/CPS/2022/003) and VEGA 2/0137/23

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Analysis of Mechanical Properties of Wire and Arc Additively Manufactured AA5087 Aluminium Alloy

Miroslav Sahul[1*], Martin Sahul[2], Ladislav Kolařík[1], Marián Pavlík[2], Vít Novák[1], Florian Pixner[3]
[1] *Faculty of Mechanical Engineering, Czech Technical University in Prague (Czech Republic)*
[2] *Faculty of Materials Science and Technology, Slovak University of Technology in Bratislava (Slovakia)*
[3] *Institute of Materials Science, Joining and Forming, Graz University of Technology (Austria)*
* miroslav.sahul@fs.cvut.cz

Abstract ID #MTFC-0891

In generally, Wire and Arc Additive Manufacturing (WAAM) is a process of metal parts production by cladding of welding beads layer by layer. It belongs to the group of directed energy deposition processes, when electric arc melts and deposits wire feedstock to fabricate elements with required shapes and dimensions [1, 2]. High deposition rates from 2 to 4 kg/h), material utilization up to 90 % and outstanding energy efficiency from 85 % to 90 % are the most important benefits of the method. In addition, compared to conventional subtractive processes such as machining the WAAM method can reduce manufacturing cost from 7 % to 69 % [3, 4]. Consequently, the WAAM processes are very popular in sectors such as automotive, aerospace, naval, oil, gas, and manufacturing industries [5]. Based on above, the research of WAAM processes is nowadays very important, because of many technological and metallurgy issues that could be encountered during the components manufacturing.

5087 aluminium alloy filler material with the diameter of 1.2 mm was suggested for building the light alloy walls. Filler material is characteristic by higher tensile strength, and the small amount of zirconium improves resistance to hot cracking. Different welding modes of Cold Metal Transfer (CMT) process were used to wire and arc additive manufacture the aluminium alloy components. The influence of welding mode on the mechanical properties of deposited components was investigated. Microhardness measurements and tensile testing of walls were used for the evaluation of mechanical properties of the components. The average microhardness of deposited walls across the wall height was very similar. The highest microhardness was measured for CMT Pulse deposited aluminium alloy wall followed by the microhardness of CMT and CMT Cycle Step built components. The highest tensile strength was recorded for the wall produced with CMT mode. The average tensile strength reached 302 MPa in such a case. Slightly lower tensile strength was measured for the component produced with CMT Pulse WAAM. The lowest tensile strength was observed in the case of walls deposited with CMT Cycle Step mode. The mentioned tensile strengths were attained for the samples cut off in the direction of overlay welding direction (horizontally cut off samples). The higher tensile strength was recorded for horizontally cut off samples in comparison to vertically cut off ones.

ACKNOWLEDGEMENTS

This work was supported by the VEGA grant agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic, project No. 1/0287/21. The paper was prepared also with the support of the Ministry of Education, Youth, and Sports of the Czech Republic.

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Resonances in Nanocomposites with Ferromagnetic Grains FeCoZr Embeded in the CaF_2 Matrix

Vitalii Bondariev*
Department of Electrical Devices and High Voltage Technology, Lublin University of Technology (Poland)
* v.bondariev@pollub.pl

Abstract ID #MTFC-0897

The paper presents the frequency and temperature dependencies of various parameters of (FeCoZr)x(CaF_2)(100-x) nanocomposite films. These films were prepared by depositing using ion-beam sputtering in a mixed argon-oxygen gas atmosphere. The focus of the study was on the phase shift angle, active part of admittance, capacitance, and dielectric loss factor tgδ.

The investigated films exhibited a "core-shell" nanostructure, where metallic FeCoZr nanoparticles were embedded in an oxygen-free dielectric matrix, forming a transparent ceramic [1-3]. After 15 minutes of annealing at a temperature of 398 K, the films with a metallic phase content of x = 62.7 at.% showed a significant "negative capacitance" effect. This effect indicated the prevalence of an inductive-like contribution to the admittance.

The observed phenomena were accompanied by two types of resonances. The first was a voltage resonance [4], typical of series conventional RLC circuits, and the second consisted of two current resonances [5], typically observed in parallel conventional RLC circuits. The voltage resonance was evident as a sharp minimum at a specific frequency fminC, where the modulus of the capacitance C(f) curves crossed zero. The two current resonances appeared as distinct minima on the conductivity σ(f) plots, occurring at θ values of θ1 = -90° and θ2 = +90°, respectively.

To explain these phenomena, a complex equivalent circuit model was proposed. This model included one series RLC circuit and two parallel RLC circuits, each with different values for their resistance, inductance, and capacitance elements. The joint analysis of the σ(f), θ(f), Cp(f), and tgδ(f) curves provided insight into the resonances, and was explained based on the previously developed AC/DC hopping model, which considered three different characteristic times of electron hopping.

The authors propose that the observed behavior and the contributions to the equivalent circuit can be attributed to the three-phase structure of (FeCoZr)-based nanoparticles. These nanoparticles consist of metallic "cores" (phase I) covered with native FeCo-based oxide "shells" containing two types of oxides (Fex_2+Co_1-x2+O crystalline oxide - phase II and α-Fe_2O_3 disordered oxide - phase III) between the metallic core and CaF_2 matrix.

ACKNOWLEDGMENTS

Participation in the 2023 IEEE 13th International Conference Nanomaterials: Application & Properties was funded by an internal grant under the Automatics, Electronics, Electrical Engineering and Space Technologies Discipline Fund.

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Functionalised High-Entropy Alloys and Coatings with Optimized Physical and Mechanical Properties in Antimicrobial and Biocorrosion Applications

Bogdan Postolnyi[1*], Radu Robert Piticescu[2], Laura Madalina Cursaru[2], Beatrice Adriana Serban[2], Dumitru Mitrica[2], Arcadii Sobetkii[2], Vladyslav Rogoz[3], Vladimir Buranich[4], Alexander Pogrebnjak[2,4]

[1] *Institute of Physics for Advanced Materials, Nanotechnology and Photonics, Faculty of Sciences, University of Porto (Portugal)*

[2] *National Research-Development Institute for Non-Ferrous and Rare Metals - IMNR (Romania)*

[3] *Thin Film Physics Division, Department of Physics, Chemistry and Biology, Linköping University (Sweden)*

[4] *Institute of Materials, Faculty of Materials Science and Technology in Trnava, Slovak University of Technology in Bratislava (Slovakia)*

*b.postolnyi@gmail.com

Abstract ID #MTFC-0898

In recent years, the antimicrobial properties of certain metals have been extensively explored for various applications. Researchers have harnessed these properties in a range of fields, including healthcare, food packaging, water treatment, and air purification. While antimicrobial coatings have emerged as a popular solution, it has been observed that some coatings experience reduced wear performance upon functionalization with antimicrobial metals. To overcome this limitation, a potential solution lies in the utilization of high-entropy alloys (HEAs) and coatings, which embed antimicrobial metals within their alloy matrix.

HEAs and coatings offer several beneficial advantages in antimicrobial applications. Potentially, these materials can exhibit excellent antimicrobial properties, effectively inhibiting the growth and spread of bacteria, fungi, and other microorganisms, and at the same time have remarkable physical and mechanical properties, such as high hardness, wear resistance, corrosion resistance, and thermal stability. This dual functionality, combining antimicrobial efficacy with desirable material properties, makes HEAs a promising candidate for various applications requiring both antimicrobial action and robust mechanical performance.

The design of HEAs and antimicrobial coatings can be significantly enhanced by leveraging machine learning methods. Researchers can efficiently screen and optimize alloy compositions by utilizing computational models and data-driven algorithms, predict material behavior, and accelerate the discovery of new HEA-based antimicrobial systems. This interdisciplinary approach, integrating materials science, chemistry, and computer science, enables the development of tailored materials with precise antimicrobial properties and enhanced performance.

This research offers a wide range of potential applications and fields where HEAs and antimicrobial coatings can be employed. Some notable examples include medical implants and devices, where the prevention of biofilm formation and infections is crucial. Similarly, the food industry can benefit from HEA-based coatings on food packaging materials to ensure food safety and extend shelf life. Other potential applications encompass water purification systems, air filtration, personal protective equipment, and touch surfaces in public spaces. The focus is on preventing biocorrosion development in multiple industries and sectors of economics. High-entropy alloys and coatings represent a promising avenue for the development of antimicrobial materials. Combining antimicrobial functionality with excellent physical and mechanical properties, these materials offer versatile applications across various fields. Moreover, the integration of machine learning techniques further enhances the design and optimization of HEAs, propelling research in this interdisciplinary field.

ACKNOWLEDGMENTS

The research is partially funded by PNRR/C9/MCID/I8, ctr. no. 760105/23.05.2023, project 58-AHEAD.

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Thin Film Deposition of Aluminum on a Silicon Substrate: Computational Modeling & Experimental Study

Rosalba Huerta[1,2*], Weiling Xia[1], Owen Bellevage[1], Benjamin Church[1], Valentine Novosad[2]
[1] *Materials Science and Engineering, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53211 (United States)*
[2] *Materials Science Division, Argonne National Laboratory, Lemont, IL 60439 (United States)*
* rosalbahuerta2027@u.northwestern.edu

Abstract ID #MTFC-0905

We computationally investigated the effect of film growth parameters on the deposition of aluminum thin films by Molecular Dynamics (MD) and Monte Carlo (MC) methods. Utilizing a Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software, the vapor deposition of aluminum atoms was simulated on the surface of a silicon substrate. By adjusting the atom energy as a function of deposition parameters using SIMTRA, we can monitor the formation of film and understand the growth process during the physical vapor deposition (PVD) process. In the case of the Al-Si system, we compare the simulated physical results to the experimental data of surface morphology. This work improves our understanding of fundamental topics, such as the growth of thin-film superconducting materials and the materials processing relevant to thin-film devices. Further analysis of the correlation between simulations and experimentally grown films allows for better application for microelectronic applications, including novel superconducting sensors, logic, memories, and low-loss high-frequency circuitry, due to their high electron conductivity and mobility, chemical stability, compatibility in technology.

ACKNOWLEDGMENTS

We would like to thank The Office of Undergraduate Research at the University of Wisconsin-Milwaukee for the SURF awards provided to the students as well as the U.S. Department of Education's Robert McNair program for their support.

TRACK 4

“NANOSCALE CHARACTERIZATION & IMAGING”

Structural and Optical Characterization of MoS_2 Nanocrystals Prepared by Green Colloidal Synthesis

Peter Hutár[1, 2*], Filip Zechel[2], Viliam Vretenár[3], Karol Végsö[4], Peter Šiffalovič[5], Milan Sýkora[2]

[1.] *Institute of Electrical Engineering SAS, Bratislava (Slovakia)*

[2.] *Laboratory for Advanced Materials, Faculty of Natural Sciences, Comenius University, Ilkovičova 8, 84104 Bratislava (Slovakia)*

[3.] *Centre for Nanodiagnostics of Materials, Faculty of Materials Science and Technology, Slovak University of Technology, Vazovova 5, 812 43 Bratislava (Slovakia)*

[4.] *Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, 84511 Bratislava (Slovakia)*

[5.] *Centre of Excellence for Advanced Materials Application, Dúbravská cesta 9, 84511 Bratislava (Slovakia)*

* peter.hutar@gmail.com

Abstract ID #NCI-608

Molybdenum disulphide (MoS2) is layered semiconductor with promising properties from electronic and optical points of view. Electronic and optical properties of MoS2 depend on dimensions and structure of the crystals. Nanoscale size MoS2 crystals have electronic structure affected also by a lateral spatial confinement and the electronic contributions from the nanocrystallites edges. Sizes distribution, shapes and edges, stimulated by the conditions of the chemical synthesis, such as nature of the precursors and reaction conditions, can significantly affect the properties of the MoS2 nanocrystals. Our investigation of the nanocrystals prepared by using various nontoxic sulphur and molybdenum precursors shows that the shape and dimensions of the resulting MoS2 nanocrystals vary to a great extent, depending on the specifics of the precursors. Position of Raman modes for set MoS2 nanocrystals suggests a significant lattice disorder. MoS2 nanocrystals prepared from different precursors differ by intensity profile, lifetime, and relative quantum yield of the photoluminescence. Number of physically and chemically active edges evolves with dimensions and structure MoS2 nanocrystals. The demonstration of a possibility to control optical and electronic properties of MoS2 nanocrystals via choice of less toxic chemical precursors opens a path to development of practical applications of MoS2 nanocrystals in areas such as advanced electronics, catalysts or chemical sensing.

ACKNOWLEDGMENTS

This work was supported by the European Union's Horizon 2020 research and innovation programme under Grant Agreement 810701, by the Slovak Research and Development Agency under Grant Agreement APVV-19-410 and Slovak Ministry of Education under grant agreement No. 1/0892/21.

Novel MFM Probe With a Disk-Shaped Magnetic Tip Apex

Ján Šoltýs[1*], Iuliia Vetrova[2], Juraj Feilhauer[2], Sergey Krylov[2], Ján Fedor[2], Tomáš Ščepka[2], Vladimír Cambel[2]

[1.] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava (Slovakia)*
[2.] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

* jan.soltys@savba.sk

Abstract ID #NCI-699

Magnetic force microscopy (MFM) is a well-established technique to investigate magnetic nano and microstructures. To improve its capability, various custom-made MFM probes have been developed. Much effort has been made to improve the spatial resolution or to reduce/increase the probe-sample interaction.

Recently we have developed a novel type of durable probe whose tip apex is not sharp, but it is equipped with a ferromagnetic disk-shaped apex (FMD tip). The interesting feature of such a tip is that its mechanical and magnetic properties are separated [1, 2]. A magnetic vortex is spontaneously created in the FMD tip and represents its ground state. The circular arrangement of the magnetic dipoles creates a closed domain state that does not generate any stray field, except for a narrow vortex core that produces an out-of-plane magnetization of the tip. Thus, the vortex core acts like a magnetically sharp nanoscale probe while the tip apex is quite large (100 - 300 nm), i.e. robust and wear-resistant.

This work is devoted to the theoretical and experimental study of the FMD tip benefits and limits. We verified its capability by scanning different magnetic structures, starting with submicron domains written in a magnetically hard sample to large domains formed on the magnetically soft sample. We evaluated the spatial resolution of the probe by scanning a high-density magnetic recording medium and found that the FMD tip provides a similar resolution to a commercial low-moment tip. It is because the narrow vortex core plays the primary role in the tip-sample magnetic interaction. However, when scanning large domains, the situation is different. The obtained MFM scans provide a different magnetic image compared to commercial CoCr tips, it highlights only boundaries between domains with opposite magnetization. We performed numerical simulations using MuMax3 and explained the reason for such imaging, which is the induced magnetization of the tip caused by the sample stray field. As a result, the MFM contrast is predominantly generated by the interaction between the sample and the induced magnetic moment rather than with the vortex core.

In summary, the FMD tip can be suitable for investigating very small domains and magnetic nanoparticles as well as for large domains when information about the shape of domains and their distribution is more important than information about the magnetization orientation. At the same time, the tip offers a long lifetime due to its robustness.

ACKNOWLEDGMENTS

The work was supported by Slovak Grant Agency VEGA (Project No. 2/0168/22), and by the ITMS (Project No. 313021T081) supported by Research & Innovation Operational Programme funded by the ERDF.

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Looking Under the Hood - Probing Degradation Mechanisms of Analog Memristors by Combination of Thin Film Spectroscopy Techniques

Boris Hudec[1] *, Che-Chia Chang[2], Tuo-Hung Hou[2]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Department of Electronics Engineering and the Institute of Electronics, National Yang Ming Chiao Tung University, Hsinchu 300, Taiwan (R.O.C.) (Taiwan)*

* boris.hudec@savba.sk

Abstract ID #NCI-714

Analysis of defects, chemistry, stoichiometry, valence and bonding states and other characteristics of thin films can be achieved using various optical and chemical, surface- or bulk-sensitive, spectroscopy techniques. Taking into account the constraints of each type of analysis, one can often puzzle together various spectroscopic data into a rather complex picture of the studied thin film material. Once the thin films of only several nm of thickness are layered on each other forming a nano-electronic device, the choice of spectroscopic techniques able to obtain data from these buried ultra-thin films and their interfaces becomes limited, and one is often left with interpretation of the electronic transport behaviour, which may be a non-trivial task without complementary spectroscopic data.

In this work we will demonstrate how various spectroscopy techniques combined can shed light onto electrical degradation of analog memristors – nano-electronic devices whose resistance can be altered by external voltage stimuli [1,2]. Memristors have several emerging application areas in computing and communications, finding use in artificial intelligence when integrated in three-dimensional crossbar arrays as artificial synapses for low-power, beyond–von Neumann architectures [3]. Other applications include random-number generation for data encryption and radiofrequency switches for mobile communications [1,2].

Although various mechanisms have been proposed for the actual resistive switching of analog memristors, it is clear that both electronic and ionic conduction phenomena are responsible for the resistance modulation [4], with a clear link to reliability issues. We will first establish which defects are responsible for memristive phenomenon in oxide films of our memristors based on combining extensive electrical characterisation data with spectroscopic ellipsometry (SE) and X-ray photoelectron spectroscopy (XPS) including the valence band spectra. Devices degraded by being repeatedly switched thousands of times - so called cycling degradation, will then be studied by combination of X-ray absorption near-edge spectroscopy (XANES), optical absorption spectroscopy (OAS) and scanning transmission electron microscopy with electron energy loss spectroscopy (STEM/EELS), establishing the overall picture of the cause of the electrical fatigue, paving the way to solutions.

ACKNOWLEDGMENTS

This work was supported by the Operational Program Integrated Infrastructure for the project: New fabrication technology of sensors, detectors and memristors for intelligent microelectronics in the 21st century, ITMS project code 313011BVN5, co-financed by the European Regional Development Fund (ERDF).

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Structural and free-Volume Characterization Y-Doped $BaTiO_3$ Ceramics

Halyna Klym*, Yuriy Kostiv
Lviv Polytechnic National University (Ukraine)

* klymha@yahoo.com

Abstract ID #NCI- 722

It is worth mentioning that $BaTiO_3$ ceramics are widely used in various applications due to their ferroelectric and piezoelectric properties. The addition of Y as a dopant has been reported to enhance these properties and improve the performance of $BaTiO_3$ ceramics in many applications.

In this study, the inner-structure properties of undoped and Y-doped $BaTiO_3$ ceramics were investigated using a combination of methods. Specifically, ceramics doped with varying amounts of Y (0.2, 0.4, 0.6, and 0.8 mol%) were sintered at 1250 ^oC, and their properties were analyzed using positron annihilation lifetime (PAL) measurements and scanning electron microscopy (SEM).

The PAL measurements were performed using an ORTEC spectrometer with a ^{22}Na source placed between two sandwiched ceramic samples. The data obtained from these measurements were analyzed using the LT computer program, and the best results were obtained using two-component fitting procedures. By accepting a two-state positron trapping model, the short lifetime (0.16 ns) was attributed to the free annihilation of positrons, which is generally observed in polycrystalline ceramic materials. This value was found to be similar to the theoretically calculated free positron lifetime in $BaTiO_3$, indicating that the ceramics had a similar free-volume defect structure to that of single-crystal $BaTiO_3$.

The value of lifetime of the second componet (0.37 ns), on the other hand, was believed to come from the annihilation of positrons at vacancy complexes formed between the oxygen vacancies and the metal ion vacancies. It was observed that lifetime of the second component decreased with the rise of Y content in $BaTiO_3$ ceramics from 0.2 to 0.6 mol%, and increased in samples with 0.8 mol% of Y. The intensity I_2 also decreased from 20 to 15%, indicating that the doping of Y resulted in a decrease in the size and amount of free-volume defects in the ceramics. This process is known as the shrinking of defects.

SEM investigations revealed that the typical ceramic samples had a grain-porous microstructure and assemblies of fractional grains. The results of this study suggest that the process of shrinking defects takes place in $BaTiO_3$ ceramics doped with Y in the range of 0.4 to 0.6 mol%. However, increasing the Y content to 0.8 mol% resulted in a weakly expressed agglomeration of free-volume defects.

Overall, this study provides valuable insights into the effects of Y doping on the inner-structure properties of $BaTiO_3$ ceramics. The combination of PAL measurements and SEM investigations allowed for a comprehensive understanding of the changes in the ceramics' defect structure as a result of Y doping, which could be useful for the development of new and improved ceramic materials.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Education and Science of Ukraine (Project No 0122U000807).

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Scanning Auger Microscopy as a Tool for Direct Characterization of 3D Elemental Distribution In Multicomponent Materials and Structures

Larysa Khomenkova[1, 2 *], Nadiia Korsunska[1], Semyon Ponomaryov[1], Yuliia Polishchuk[1], Kostiantin Kozoriz[1], Maryna Khrypko[1], Lyudmyla Melnichuk[3], Oleksandr Melnichuk[3]

[1.] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine (Ukraine)*

[2.] *National university "Kyiv-Mohyla academy" (Ukraine)*

[3.] *Mykola Gogol State University of Nizhyn, 2 Hrafska str., Nizhyn 16600, Ukraine (Ukraine)*

* khomen@ukr.net

Abstract ID #NCI-781

The application of multicomponent materials requires the monitoring of their optical, luminescent and electrical properties being supported by the structural characterization and the analysis of chemical composition. The combination of X-ray diffraction, Raman scattering spectroscopy and infrared reflection spectroscopy provides information about the morphology and crystalline structure but their spatial resolution is low enough. Transmission electron microscopy permits to get insight on the local crystalline structure, but it needs complicated procedures for specimen preparation. Besides, the interpretation of the obtained results depends strongly on the spatial matching of averaging composition and specimen orientation. Furthermore, for multicomponent nanoscaled polycrystalline materials, the analysis of elemental distribution meets the difficulty due to the overlapping of the grains with different sizes and different chemical composition. Thus, to investigate polycrystalline materials, the application of surface sensitive approach with high spatial resolution is required.

The combination of Auger electron spectroscopy and high-resolution scanning electron microscopy can overcome these problems. This approach (called hereafter as SAM) was successfully used by us earlier for the analysis of spatial distribution of Si and Ge inside GeSi nanoislands grown on Si substrate [1]. The Auger spectra were recorded using an effective control of thermal drift of the analyzed site by regular electronic correction of the GeSi nanoisland position on the SEM image taken from the corresponding surface area. The chemical composition was analyzed with the lateral resolution of about 3–5 nm and the depth resolution of about 1 nm.

Recently, the SAM approach was applied to monitor the chemical composition in ZnO and ZnO:Mn ceramics [2]. The pronounced Zn accumulation at the grain boundaries upon ceramics sintering was revealed. This effect was found to be dependent on the preliminary powder milling as well as on the pressure value applied upon their compacting [2].

In present report, we demonstrate the SAM ability to monitor the variation of spatial element distribution in the ceramic materials and thin films. At first, the effect of the compacting pressure and sintering conditions on the structural and compositional properties of MgxZn1-xO ($0 \leqslant x \leqslant 1$) ceramics will be presented. These results will be compared with those obtained by traditional spectroscopic methods. Simultaneous formation of (Mg,Zn)O cubic and hexagonal solid solutions will be shown. However, it will be emphased that the hexagonal grains have homogeneous Mg distribution, while the gradual Zn distribution will be shown for cubic grains of solid solution. Then, the application of the SAM approach for the characterization of thin films based on metal oxides (ZnO, HfO_2, Al_2O_3, etc.) will be also demonstrated and the observed pecularities of such materials will be discussed.

ACKNOWLEDGMENTS

This work was partly supported by the National Research Fund of Ukraine from the state budget, project 2020.02/0380 "Structural transformations and nonequilibrium electronic processes in broadband oxides and their solid solutions."

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Analyzing and Assembling Layered Materials, Atom by Atom and Layer by Layer, in 2D and 3D

Jannik C. Meyer[1, 2, 3*], Christoph Hofer[1, 2, 4], Jonas Haas[1, 2], Jani Kotakoski[3], Toma Susi[3], Clemens Mangler[3], Viera Skákalová[5, 6, 3], Andreas Mittelberger[4], Giacomo Argentero[4], Mohammad R. A. Monazam[4], Christian Kramberger-Kaplan[4], Xiao Wang[7], Kai Braun[8]

[1.] *Institute of Applied Physics, Eberhard Karls University of Tuebingen, Auf der Morgenstelle 10, D-72076, Tuebingen (Germany)*
[2.] *Natural and Medical Sciences Institute at the University of Tuebingen, Markwiesenstr. 55, D-72770 Reutlingen (Germany)*
[3.] *Faculty of Physics, University of Vienna, Vienna (Austria)*
[4.] *University of Vienna, Faculty of Physics, Boltzmanng. 5, 1090 Vienna (Austria)*
[5.] *Institute of Electrical Engineering and CEMEA SAS, Bratislava (Slovakia)*
[6.] *Danubia NanoTech s.r.o., Bratislava (Slovakia)*
[7.] *School of Physics and Electronics, Hunan University, Changsha, Hunan 410082 (China)*
[8.] *Institute of Physical and Theoretical Chemistry, Eberhard Karls University of Tübingen, Auf der Morgenstelle 10, D-72076, Tübingen (Germany)*

* jannik.meyer@uni-tuebingen.de

Abstract ID #NCI-874

Aberration-corrected electron microscopy is emerging as a versatile tool not only for analyzing, but more recently also for manipulating materials down to the level of single atoms. I will discuss both of these aspects and present some of our recent developments in the context of layered, two-dimensional materials: On the analysis side, we developed means to identify the 3D atomic configuration of defects, grain boundaries or impurities, from only two exposures of the same structures [1, 2]. The same approach, combined with the simple dependence of the intensity in annular dark field scanning transmission electron microscopy images on the atomic number provides (to some extent) chemical information about the sample, and hence allows an elemental identification in the case of light-element single-layer samples [3]. However, the intensity of individual atoms and atomic columns is affected by residual aberrations and the confidence of an identification is limited by the available signal to noise. We show that matching a simulation to an experimental image by iterative optimization provides a reliable analysis of atomic intensities even in presence of residual non-round aberrations [4]. This is of particular relevance for analyzing moderately beam-sensitive materials, such as most 2D materials, where the limited sample stability often makes it difficult to obtain spectroscopic information at atomic resolution. Towards an atomic-level manipulation, I will present a recent development where we combine spatially controlled modifications of 2D materials, using focused electron irradiation or electron beam induced etching, with the layer-by-layer assembly of van der Waals heterostructures [5]. A new transfer and assembly process makes it possible to stack the layers under observation in an electron microscope, such that pre-patterned features can be aligned to each other. The aligned stacking of individually patterned 2D materials layers can be considered as a form of 3D printing, where each layer is only one or a few atoms thick, and features within each layer can be defined with a nm-scale resolution.

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TRACK 5
“NANOPHOTONICS”

Influence of Dispersion in Liquid Crystal on Optical Properties of Carbocyanine Dye J-Aggregates

Oleksandr Sorokin *, Iryna Grankina, Oleksandr Samoilov, Natalia Kasian, Svitlana Hrankina, Longin Lisetski, Svetlana Yefimova
Institute for Scintillation Materials, NAS of Ukraine (Ukraine)

* sorokin@isma.kharkov.ua

Abstract ID #NP-534

In recent years, liquid crystals have been used more and more widely as host matrices for the introduction and dispersion of various inorganic and organic nanoparticles, both in fundamental studies and to obtain new composite nanomaterials. In particular, due to the unique combination of optical and anisotropic properties, luminescent liquid crystals are of great interest from the point of view of optoelectronic applications. In condensed phases, they can organize with crystalline order, leading to, for example, attractive charge transport properties, while they retain fluidity, which provides the self-healing ability and dynamic properties. Furthermore, their anisotropic organization is particularly interesting for applications with polarised light.

However, traditional luminescent liquid crystals often suffer from fluorescence quenching caused by aggregation, which significantly limits their further use. One of the approaches to overcome this problem is the use of aggregation-induced emission. An important kind of luminescent aggregate is J-aggregates, which are low-dimensional molecular crystals of some types of organic dyes, such as cyanines or perylene derivatives. Due to the excitonic nature of their electronic excitations and 1D or 2D structure, the optical properties of J-aggregates differ significantly from the properties of individual molecules or bulk crystals.

We report the formation of J-aggregates of the anionic cyanine dye TDBC in a nematic liquid crystal 5CB matrix with analysis of optical-luminescent and electro-optical properties. Unlike water solution, the TDBC J-aggregates show a rather long lifetime and high photostability in the nematic matrix. The electro-optical characteristics of the LC matrix are substantially modified, with the Fredericks transition threshold slightly increased, which is, on the other hand, accompanied by the improvement of the optical contrast. Only a minor effect of the forming J-aggregates on the molecular order of the LC structure could be noted.

ACKNOWLEDGMENTS

The authors thank the Armed Forces of Ukraine for the opportunity to prepare the work for publishing. OS expresses sincere gratitude to Dr. Franziska Fennel from the University of Rostock for the invaluable help.

Luminescence Alteration of Converted Trivalent Europium Ions Doped Tungsten Sulfide Semiconductor Nanomaterials for Optical Applications

Namrata Pachauri *, Sri Sivakumar
Indian Institute of Technology Kanpur (India)

* namratap@iitk.ac.in

Abstract ID #NP-541

This work reports the host sensitized luminescence by the incorporation of europium lanthanide ions (Eu+3) into tungsten oxide (WO3) semiconductor nanomaterials (SCNMs) which further converted into sulfide materials for the optical applications. Eu+3 doped WO3 SCNMs was prepared with varying concentration of Eu+3 by novel and easy coprecipitation method at very low temperature 90 C for 3hrs, subsequently converted into WS2/Eu+3 semiconductor nanomaterials. Doping of lanthanide ion can assist in transferring energy from the host to the activator Ln+3 ions to produce bright luminescence. X-ray diffraction spectroscopy (XRD), X-ray photoelectron spectroscopy (XPS) and UV-Vis spectroscopy data were confirmed the successful synthesis of the WS2/Eu+3 SCNMs. Morphology of the synthesized SCNMs was observed by the TEM images and quantitative presence of each element was supported by the elemental mapping results. The photoluminescence studies have been supported the excitation of Eu+3 ions via energy transfer from the host (WS2 SCNMs) to Eu+3 ions. Thus, altered optical properties of WS2 SCNMs can be used in photodetectors, light-emitting diodes (LEDs) etc.

ACKNOWLEDGMENTS

We are grateful to Indian Institute of Technology Kanpur for providing funding and facility for research.

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Improving the Stability of Carbocyanine J-Aggregates in Layered Polymer Films

Polina Pisklova[1, 2*], Johannes Krause[2], Steffen Wolter[2], Tobias Korn[2], Svetlana Yefimova[1], Oleksandr Sorokin[1], Stefan Lochbrunner[2]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *Institute for Physics, University of Rostock (Germany)*

* polinkapisklova@gmail.com

Abstract ID #NP-576

J-aggregates are highly ordered nanostructures of non-covalently coupled dyes such as cyanines, porphyrins, merocyanines, perylenes, and others. Due to the translational symmetry within the molecular chains of a J-aggregate, the electronic excitations of the monomers are delocalized over several chain segments, and molecular (Frenkel) excitons are formed. The distinctive feature of J-aggregates is the J-band which results from electric dipole transitions into the low-energy edge of the exciton band.

J-aggregates exhibit many unique spectroscopic properties, which are distinctly different from those of the individual molecules constituting the aggregates: very narrow absorption and fluorescence line widths, near-resonant fluorescence, large extinction coefficients, giant third-order optical nonlinearities, exciton superradiance. Thus, they are ideal candidates for novel photonic materials, especially for thin-film applications. Unfortunately, pure aggregate films are often not stable enough. Polymer-based thin films with incorporated J-aggregates could be more durable and might be an attractive alternative [1].

One of the methods to form J-aggregates in polymer film is a layer-by-layer assembly. In this technique, alternative multilayered polymer films can be deposited using electrostatic attraction onto an electrically charged substrate by its sequential dipping in aqueous solutions of polycations and polyanions [1]. The advantage of the method is the controlled assembly of the necessary combination of studied species separated by a spacer of defined thickness. However, the solution-based process of the film preparation and their extremely small thickness (approximately 2 nm for one polymer layer) can result in high penetrability of molecular oxygen, which is one of the main reasons for organic fluorophores photodegradation.

In the present report, the stability of TDBC J-aggregates in layered polymer films was studied using absorption and fluorescence spectroscopy. It was found, that the J-aggregates in pure films of polycation PDDA are very unstable. The additional deposition of an other polymer like polyvinyl alcohol over the prepared films increases the stability at least 3 times. However, much better results were obtained by physical vapor deposition of thin metallic films (20 nm gold and 3 nm titanium) over TDBC J-aggregates in PDDA films. Such a structure is promising for photonic applications of thin film J-aggregates.

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Interaction Between J-Aggregates of Cyanine Dyes in Layered Polymer Films

Iryna Ropakova[1*], Polina Pisklova[1, 2], Svetlana Yefimova[1], Stefan Lochbrunner[2], Oleksandr Sorokin[1]
[1.] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2.] *Institute for Physics, University of Rostock (Germany)*

* adelma@ukr.net

Abstract ID #NP-587

J-aggregates are highly ordered nanostructures of non-covalently coupled dyes such as cyanines, porphyrins, merocyanines, perylenes, and others. Due to the translational symmetry within the molecular chains of a J-aggregate, the electronic excitations of the monomers are delocalized over several chain segments, and molecular (Frenkel) excitons are formed. The distinctive feature of J-aggregates is the J-band, which results from electric dipole transitions into the low-energy edge of the exciton band.

J-aggregates exhibit many unique spectroscopic properties, which are distinctly different from those of the individual molecules constituting the aggregates: very narrow absorption and fluorescence line widths, near-resonant fluorescence, large extinction coefficients, giant third-order optical nonlinearities, exciton superradiance. Thus, they are ideal candidates for novel photonic materials, especially for thin-film applications. J-aggregates formed in thin polymer film may support surface exciton-polariton modes and, hence, concentrate the electromagnetic field at optical frequencies like metallic nanoparticles. As a result, J-aggregates may enhance fluorescence for monomeric dyes located in the aggregates' vicinity [1].

In the present report, the interaction of TDBC and TCC J-aggregates in layered polymer films was studied using stationary and time-resolved optical spectroscopy. It was found, that efficient energy transfer can be achieved with TDBC J-aggregates as energy donors and TCC J-aggregates as energy acceptors at a minimal distance between them [2]. The interactions of surface exciton-polaritons in these J-aggregates are supposed to lead to increasing fluorescence intensities and lifetimes for both aggregates. The distance dependence of the J-aggregate interaction was studied and is discussed in the frame of surface exciton-polaritons and their influence.

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Electrical Noise In ZnO Thin Films Obtained By the PLD Method

Ihor Virt[1*], Mariush Bester[2], Bogumił - Cieniek[2], Piotr - Potera[2], Andrij Lozynsyi[1]
[1.] *Drohobych State Pedagogical University I.Franko (Ukraine)*
[2.] *University of Rzeszow (Poland)*

* isvirt@email.ua

Abstract ID #NP-770

The article presents the results of studies of the noise characteristics of zinc oxide thin films grown by laser deposition [1]. X-ray diffractograms were studied and the crystal structure of the films was determined. The noise characteristics were studied under illumination with band-gap excitation, as well as without illumination. The influence of deep traps and their concentration was evaluated.

Cobalt-doped zinc oxide thin films were obtained by pulsed laser deposition (PLD) with various laser ablation parameters of ZnO targets. Films with a mosaic monocrystalline structure with a thickness of about 50-500 nm were obtained. Non-equilibrium effects, in particular photoeffects, in high-resistance ZnO films doped with Co were investigated. The low-frequency noise (0.01÷100 kHz) of the manufactured UV photoreceptor ZnO on Al_2O_3 was investigated and methods of its suppression were proposed. I used a DSO-2250 USB oscilloscope with a 20 ms window, 20 μs sampling. It was found that dark current noise and photocurrent noise have different mechanisms. The total current noise spectrum can be represented as the sum of three components: thermal, generation-recombination, and excessive 1/f. Hooge's constant varies within 5÷0.05 depending on the number of carriers created. Illumination of samples from the region of main light absorption (non-equilibrium process) leads to an increase in the G-R noise contribution. This contribution has a lasting impact. Zone-zone excitation illumination causes characteristic G-R noise with a Lorentzian relaxation time of 9 μs. The influence of deep traps and their concentration was estimated and the concentration of traps $N_t \sim 4 \cdot 10^{17}$ cm^{-3} was determined [2,3].

Photoelectric characteristics were measured: current coefficient, ampere-watt sensitivity in the UV range, sensitivity to NEP, photocurrent kinetics. The current ratio of the illuminated and non-illuminated sample was $\sim 10^3$.

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Enhancement of Optical Properties of GaAs Quantum well Cap Layer

Jirarut Joonhuay [*], Paphavee van Dommelen
Division of Physical Science, Faculty of Science, Prince of Songkla University (Thailand)

* 6510230007@email.psu.ac.th

Abstract ID #NP-775

Localized surface plasmon resonance (LSPR) of cuboid gold nanoparticle (AuNP) on the GaAs cap layer of the GaAs/AlGaAs quantum well (QW) is investigated by using the 3-D finite element method (FEM). Increasing the lateral dimension (L) of AuNP can boost the extinction cross sections and affect the red shift of wavelength. Furthermore, we include the effect of distance between the GaAs cap layer and AuNP in terms of nanogap between these two surfaces, and the results indicate that this tiny gap can increase the intense electric field intensity near AuNP, also known as a hot spot, under the appropriate frequency. The modulation of the electric field surrounding AuNP in relation to the GaAs refractive index can optimize the operating wavelength and output efficiency of nanostructures. This theoretical analysis can serve as a reference for optimization without needing refabrication of a nanostructure used as a near-infrared laser or detector.

ACKNOWLEDGMENTS

This research has received funding support from the NSRF via the Program Management Unit for Human Resources & Institutional Development, Research and Innovation [grant number B05F650024], and the Development and Promotion of Science and Technology Talents Project (DPST).

Plasmonic Au Nanotube Array Absorber Via Template-Assisted Secondary Deposition for Solar Energy Application

Hak-Jong Choi*
Korea Institute of Machinery and Materials (Republic of Korea)

* hakjong_choi@kimm.re.kr

Abstract ID #NP-857

Plasmonic nanostructures offer a promising opportunity to improve the various applications such as solar energy conversion system, optical sensor, super resolution imaging, and photonic devices.[1-2] Especially, plasmonics can enhance an efficiency of solar energy conversion by controlling scattering, hot electron generation, and locally concentrated electromagnetic field. In order to improve the performance of solar devices, various plasmonic nanostructures, including nanodot, nanohole, nanocone, and nanowire, were already fabricated and studied using a lot of methods such as porous aluminum template, e-beam lithography, photolithography, nanoimprint lithography, and so on.[3]

In this study, we develop the fabrication method for plasmonic Au nanotube array for broadband absorption using nanoimprint lithography and secondary sputtering process, which can control the size and shape of Au nanotube. Briefly, nanohole pattern were fabricated on polymer coated Au/glass substrate using direct patterning of hydrogen silsesquioxane (HSQ).[4] Then, HSQ pattern was transferred on polymer layer using reactive ion etching. After that, exposed Au film was etched using low-energy Ar ion milling. Then, etched Au was simultaneously deposited on side wall of polymer pattern. Finally, HSQ pattern and polymer layer were removed using chemical etching process and Au nanotube array were successfully fabricate on glass substrate, as shown in Figure 1. The Au nanotube array were simulated using finite differential time domain (FDTD) method and characterized using optical analyzer such as UV-Vis spectrometer and ellipsometer. Then, high absorption property was observed in Figure 2. These structure were adapted in solar energy conversion system like photoelectrochemical device and thin film organic solar cell. Then, we confirmed the improvement of the solar energy conversion devices due to their excellent optical properties.

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Environmentally-conscious and Cost-beneficial Selective Extraction of Single-walled Carbon Nanotubes by Conjugated Polymers

Patrycja Taborowska[1*], Andrzej Dzienia[2, 3], Dawid Janas[2]
[1] *Silesian University of Technology, Faculty of Chemistry (Poland)*
[2] *Department of Chemistry, Silesian University of Technology, B. Krzywoustego 4, Gliwice (Poland)*
[3] *Institute of Materials Engineering, University of Silesia in Katowice, Bankowa 12, 40-007 Katowice (Poland)*

* patrycja.taborowska@polsl.pl

Abstract ID #NP-865

As synthesized single-walled carbon nanotubes (SWCNTs) material is always a mix of species with different electrical and optical properties, so for some applications post-process sorting is necessary [1]. Conjugated polymer (CP) extraction in organic solvent allows to effectively isolate SWCNT species of different diameters, conductivity type or even chiralities. The method is relatively simple as it is based on only two steps: sonication and centrifugation, during which polymer chains wrap and isolate SWCNTs of preferred type [2]. The selectivity towards single chirality can be as high as 99% but the yield of single extraction is often not satisfactory, and this is why a method of re-using SWCNT source material is implemented lately [3,4].

Here two systems of multiple close to monochiral extractions were developed and monitored with an attempt to re-use both the post-process SWCNT material and used conductive polymer. In the former case, we discovered a never previously reported gradual process of surface degradation that cannot be easily reversed. Regarding the latter, we noticed that when a polymer of moderate to high molecular weight is used, it can be reused without loss of selectivity and performance after simple washing from the nanocomposite.

Presented results are a step towards large scale extraction of monochiral SWCNT material, providing more understanding on process parameters and mechanism of selective extraction by CPs. The material can further be used for optoelectronic emitters and sensors, where it is important to use monochiral SWCNTs as it allows to effectively tune bandgap, increase sensing sensitivity and resolution or enable choice of the preferential resonance frequency. Hence, the development of simple and efficient methods of sorting SWCNTs by chirality presented in this contribution considerably advance the utilization of SWCNTs for these fields of exploitation.

ACKNOWLEDGMENTS

The authors would like to thank the National Science Centre, Poland (under the SONATA program, Grant agreement UMO-2020/39/D/ST5/00285) for supporting the research.

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Solvatochromism of Single-Walled Carbon Nanotubes Suspended In Various Organic Media

Dominik Just[1*], Andrzej Dzienia[1, 2], Dawid Janas[1]
[1.] *Department of Chemistry, Silesian University of Technology, B. Krzywoustego 4, Gliwice (Poland)*
[2.] *Institute of Materials Engineering, University of Silesia in Katowice, Bankowa 12, 40-007 Katowice (Poland)*

* dominik.just@polsl.pl

Abstract ID #NP-867

Solvatochromism refers to the change of optical properties of a given material due to a modification of the properties of the solvent or, more generally, the environment in which they are analyzed [1-3]. The characteristics of nanomaterials are most substantially affected by this phenomenon because of their strong structure-property relationship. Single-walled carbon nanotubes (SWCNTs), in particular, are very sensitive to the local environment, so they are envisioned as next-generation sensors for many external stimuli. Yet, surprisingly, the way how the environment influences their characteristics is poorly understood. The reason for this state of affairs is caused by the scarcity of structurally-homogeneous (SWCNTs), which can be obtained by a handful of techniques nowadays. One of the most promising approaches in this area is the so-called conjugated polymer extraction (CPE), which can suspend SWCNTs in organic solvents selectively [4-5]. However, the impact of these solvents on the optical properties of the harvested nanocarbon material remains unresolved.

In this work, we tackled the above-mentioned problem by conducting CPE process of SWCNTs in various organic solvents using fluorene-based polymers and copolymers. The systems were carefully selected to create monochiral suspensions allowing for a thorough study of the effect of the solvent on a given SWCNT species. Complex interactions between polymer structure, SWCNT chirality and solvent properties were elucidated, leading to the formulation of an accurate solvatochromism mechanism in SWCNTs. In-depth experimental and theoretical studies have shown that in the case of SWCNTs solubilized in CPE, the solvatochromic shifts closely depend on the assignment of particular chiral types to modes and families that experience the strain exerted by the polymer chains in different ways.

ACKNOWLEDGMENTS

The authors would like to thank the National Science Centre, Poland (under the SONATA program, Grant agreement UMO-2020/39/D/ST5/00285) for supporting the research.

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TRACK 6

“TRANSPORT PROPERTIES IN NANOSCALE SYSTEMS”

Asymmetric Magnetoresistance of Single-Walled Carbon Nanotubes Filled By Nickel

Denys Shpylka*, Iryna Ovsiienko, Tetiana Len, Liudmyla Matzui, Yuriy Prylutskyy, Tetiana Tsaregradskaya
Taras Shevchenko National University of Kyiv (Ukraine)

* denys8600@ukr.net

Abstract ID #TPNS-475

In the work the results of magnetoresistance research in single-walled carbon nanotubes (SWCNTs) filled with nickel are presented. SWCNTs have been obtained by the electric arc method during the evaporation of a graphite electrode (anode) with a nickel catalyst pressed into it in a helium atmosphere. According to detailed structural and phase studies [1], the obtained single-walled carbon tubes with a diameter (1.4 – 2) nm contain particles of nickel up to 1.6 nm in size in the inner cavity.

To measure the magnetoresistance the bulk specimens in the form of rectangular parallelepipeds have been made from powder of SWCNTs by cold pressing using polyvinyl acetate (20 % mass) as a binder. In the bulk specimen, the carbon nanotubes were oriented in such a way that the axis of the tubes lies mainly in a plane perpendicular to the pressing direction.

The investigations of magnetoresistance have been carried in the temperature interval (77 – 293) K and magnetic field up to 2.5 T. In all experiments, the current was passed through the bulk specimen in the direction of the long axis of the specimen. At the same time, the direction of the magnetic field through the specimen changed. The dependences of the SWCNTs bulk specimen resistance on the applied magnetic field at the angles between the field direction and the current direction through the specimen 00 (parallel geometry), 300, 600 and 900 (perpendicular orientation) have been obtained.

Conducted studies have revealed a some features in the field dependences of magnetoresistance $\Delta\rho/\rho(B)$ for different orientations of the magnetic field relative to the current through the bulk specimen. First, there is no hysteresis in the field dependences of magnetoresistance at mutual orientation angles of 00, 300, and 600, which was found, for example, for CNTs with iron. Pronounced hysteresis is observed only in the dependence $\Delta\rho/\rho(B)$ of the magnetoresistance at the perpendicular geometry of the experiment, while the magnetoresistance does not reach saturation in fields up to 2.5 T. Second, magnetoresistance is not symmetrical with respect to the direction of the magnetic field through the specimen. At the same time, the difference in the magnitude of magnetoresistance in the positive and negative directions of the magnetic field depends on the geometry of the experiments. The relative difference between the "negative" and "positive" branches of the magnetoresistance is the largest at the parallel geometry (177%). As the angle between magnetic field and current direction increases, this difference decreases.

The asymmetric magnetoresistance found in the SWCNTs with nickel is explained within the terms of the Segal's model [2], according to which the presence of small magnetic phase inclusions in the nonmagnetic matrix causes inhomogeneity of transverse Hall voltages. This, in turn, leads to the asymmetry of the magnetoresistance relative to the direction of the magnetic field.

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Proximity Induced Spin Currents and Spin-Orbit Torques In Graphene On 1t-Tas2

Maedeh Rassekh[1] *, Marko Milivojević[2], Martin Gmitra[1, 3]
[1.] *Institute of Physics, Pavol Jozef Šafárik University in Košice (Slovakia)*
[2.] *Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia (Slovakia)*
[3.] *Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)*

* maedeh.rassekh@upjs.sk

Abstract ID #TPNS-571

Charge-spin interconversion provides a unique way to generate spin current and spin-orbit torque, which are essential for the development of spintronic devices [1]. The proximity of a transition-metal dichalcogenide (TMD) to graphene can have a profound effect on the magnetism and spin texture of graphene. This effect comes from the induced spin-orbit coupling (SOC) of the TMD, which complements the high-quality charge and spin transport of graphene [2, 3]. One of the most promising materials for SOT research is 1T-TaS2 which comprises both strong SOC and spontaneous in-plane magnetization. When a layer of graphene is placed on top of 1T-TaS2, a SOC and exchange interaction is proximitized to graphene electronic structure. This enables generation of spin-orbit torques (SOT) [4] without a need of spin-polarized current injection by a ferromagnet.

Using an effective tight-binding model [5] combined with quantum transport calculations, we show that the flow of an unpolarized current across a single layer of graphene proximitized with 1T-TaS2 will exhibit SOT driven by the unpolarized injected charge current. Our results show an overall spin accumulation for the spin component perpendicular to the plane. Remarkably, the sign of the accumulated spin density depends on the electron or hole nature of the injected current. On the other hand, for the injected electrons with spins along the longitudinal direction, a spin separation is observed perpendicular to the current direction, which is the signature of the spin Hall effect. Interestingly, these results are independent of stacking type. The subsequent interaction of the current-induced spins with the 1T-TaS2 layer generates SOT. Our findings shed new light on the fundamental behavior of spin currents and SOT in graphene-TaS2 heterostructures and highlight the potential of these materials for developing spintronic devices.

ACKNOWLEDGMENTS

This work was supported by the Slovak Research and Development Agency provided under Contract No. APVV-SK-CZ-RD-21-0114, SASPRO 2 COFUND Marie Sklodowska-Curie grant agreement No. 945478, VEGA 1/0105/20 and Slovak Academy of Sciences project IMPULZ IM-2021-42 and project FLAG ERA JTC 2021 2DSOTECH.

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Computational Study of the Thermal Transport Properties of Hollow-Core Si

Vasyl Kuryliuk, Viktoria Shevchenko*
Taras Shevchenko National University of Kyiv (Ukraine)

* shevchenko@univ.kiev.ua

Abstract ID #TPNS-611

Due to their unique phonon transport properties, silicon nanowires are an attractive material for use in the thermal management of nanoelectronics and optoelectronics [1,2]. The scattering of thermal vibrations on the surface of Si nanowires leads to a significant reduction in thermal conductivity compared to bulk silicon, which finds application in thermoelectric elements. Further progress in these areas requires new research to explore methods of reducing the thermal conductivity of nanowires. One possible option in this direction could be the use of silicon nanowires with hollow-core morphology [3,4]. Such nanowires have a higher surface-to-volume ratio, which results in more intense phonon scattering on the surfaces of the structure. Understanding the thermal transport properties of these nanowires is crucial for designing efficient thermal management devices. In this study, we investigate the thermal conductivity of hollow-core silicon nanowires using the molecular dynamics method, depending on the wall thickness. The temperature influence on phonon transport processes is also studied. Our results show that the thermal conductivity of hollow-core Si nanowires is highly dependent on the wall thickness. We observe a significant decrease in thermal conductivity as the wall thickness decreases, which can be attributed to the increased phonon scattering at the core-shell interface. To explain the obtained dependencies, the density of vibrational states and phonon participation ratio is analyzed in detail. Our study provides insights into the thermal transport properties of hollow-core silicon nanowires and highlights the importance of considering nanowire geometry in designing efficient thermal management devices. Our results can also guide the development of new materials with tailored thermal transport properties for specific applications.

ACKNOWLEDGMENTS

We gratefully acknowledge the financial support from the National Research Foundation of Ukraine for supporting this work by Grant NO. 2020.02/0067.

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Electrical Properties of Mo-W-C Nanocomposite Films

Piotr Gałaszkiewicz[1*], Pawel Zukowski[1], Tomasz Koltunowicz[1], Alexander Pogrebnjak[2, 3], Kateryna Smyrnova[4], Martin Sahul[5], Vitalii Bondariev[6]

[1.] *Lublin University of Technology (Poland)*
[2.] *Sumy State University (Ukraine)*
[3.] *Faculty of Material Science and Technology in Trnava, Slovak University of Technology in Bratislava, Trnava (Slovakia)*
[4.] *Slovak University of Technology in Bratislava (Slovakia)*
[5.] *Faculty of Materials Science and Technology, Slovak University of Technology in Bratislava (Slovakia)*
[6.] *Department of Electrical Devices and High Voltage Technology, Lublin University of Technology (Poland)*

* p.galaszkiewicz@pollub.pl

Abstract ID #TPNS- 621

Transition metal carbides due to their excellent electrical, mechanical, and thermal properties, and the possibility of manipulating them through changes in the chemical composition, are of great interest nowadays [1,2].

This paper presents the results of a study of the alternating electrical properties of Mo-W-C composition layers. The layers were prepared using a two-source magnetron sputtering method. Structural studies showed that the obtained layers are nanocomposites consisting of metal carbide nanoparticles incorporated into an amorphous carbon matrix with a thickness of approximately 950 nm. The alternating-current electrical properties of the films were measured in the temperature range from 20 K to 375 K in the frequency range from 50 Hz to 2 MHz.

Two nanocomposite layers S1 and S4 were selected for conductivity and dielectric permeability studies. Layer S1 contained 100% of $(Mo_2+W_2)C$ nanoparticles, while layer S4 contained 28 % of $(Mo_2+W_2)C$ and 72 % of a MoWC nanoparticles. Nano-grained structure of the layers supports the occurrence of hopping conductivity [3]. To analyse the results obtained, a model of DC and AC step conductivity based on the quantum mechanical phenomenon of electron tunneling between nanometer-sized potential wells was used [4].

The temperature-frequency characteristics of the conductivity and the frequency factor α(f) were determined for both layers. For both samples, there were two mechanisms observed to influence the conductivity and α(f) factor values, high-frequency and low-frequency. From the maxima on the α(f) factor characteristics, the values of relaxation time were calculated, and in terms of the occurrence of the low-frequency stage, the temperature dependence of the relaxation time was determined, and from this, the activation energy of the relaxation time was determined to be $\Delta E1 \approx 0.316$ eV for layer S1 and $\Delta E4 \approx 0.333$ eV for layer S4. Based on the dielectric permeability of the layers, the potential energy of the dipoles was determined to be (0.07 ± 0.004) eV. On this basis, the average distance between carbide nanoparticles (distance over which electrons tunnel) was calculated, which was (3.4±0.2) nm.

ACKNOWLEDGMENTS

Participation in the 2023 IEEE 13th International Conference Nanomaterials: Application & Properties was funded by a grant Szkola Doktorska-Grant -Piotr Gałaszkiewicz

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Annealing Effect on Bi_2Te_3 Topological Surface States as Seen From Magnetoresistance Probed at Sub-Kelvin Temperatures

Maciej Chrobak[1, 2*], Kamil Nowak[1], Michał Jurczyszyn[2], Andrii Naumov[3], Marek Przybylski[1]

[1.] *Faculty of Physics and Applied Computer Science, AGH University of Krakow, 30-059 Krakow, Poland (Poland)*
[2.] *Academic Centre for Materials and Nanotechnology, AGH University of Krakow, 30-059 Krakow, Poland (Poland)*
[3.] *AGH University of Krakow, Academic Centre for Materials and Nanotechnology, al. Mickiewicza 30, 30-059 Krakow, Poland (Poland)*

* mchrobak@agh.edu.pl

Abstract ID #TPNS-682

3D topological insulators (TIs), such as bismuth telluride (Bi_2Te_3) and bismuth selenide (Bi_2Se_3), can be characterized as materials of a semiconducting volume and a conductive surface. These metallic boundaries originate as a consequence of a topologically nontrivial electronic structure resulting from the strong spin-orbit coupling. The surface states form characteristic Dirac cones with linear dispersion relation. Such an electronic structure makes TIs a promising candidate both for research on unique phenomena related to their non-trivial topology and for potential applications. Although many issues regarding TIs have been clarified in recent years, it is still an open question how annealing affects the surface states.

We report on magnetoresistance studies that include Shubnikov-de-Haas (SdH) oscillations, scanning tunneling microscopy (STM), and scanning tunneling spectroscopy (STS) of Bi_2Te_3 single crystals unheated and exposed to a high temperature.

All the tested samples reveal SdH oscillations, which prove that a long-range crystallographic order is preserved after annealing. We can distinguish two characteristic frequencies of quantum oscillations. The Landau-level fan diagram analysis confirms that the dominating SdH oscillations (with a frequency of 21.6 T) can be attributed to the topological surface states (a Berry phase equal to π). The frequency increases with increasing annealing temperature as a result of increasing the carrier concentration, which is confirmed by the Hall effect measurements. The parameters of these oscillations suggest that annealing deteriorates the surface states while improving the volume conductivity (residual resistance decreases with annealing temperature). On the other hand, the frequency of the other contributing oscillations (67 T), attributed to the volume electronic states, remains unchanged after annealing although the contribution of these oscillations increases slightly with increasing annealing temperature.

The high-resolution STM images confirm the results of the SdH oscillations. For the annealed samples, significant changes at the sample's surface are observed, which is manifested by the occurrence of a new phase of a height corresponding to a fraction of the height of a single quintuple layer. The STS spectra measured at the affected area show remarkable changes in the electronic structure compared to the unaffected surface: the linear dispersion relation disappears.

ACKNOWLEDGMENTS

Research project partly supported by program "Excellence initiative - research university" for the AGH University of Science and Technology.

K. N. was partly supported by the EU Project POWR.03.02.00-00-I004/16.

TRACK 7

"NANOMAGNETISM & MAGNETIC MATERIALS"

Probabilistic Computing with Antiferromagnetic Spin Hall Oscillators

Denys Slobodianiuk*, Oleksandr Prokopenko
Taras Shevchenko National University of Kyiv (Ukraine)
* denslobod@ukr.net

Abstract ID #NMM-0495

Antiferromagnetic (AFM) spintronics is a promising and emerging branch of spintronics based on the utilization of ultra-fast magnetization dynamics in antiferromagnets (AFMs), which have two or more magnetic sublattices forming a magnetically-compensated material. Spintronic devices based on AFMs have operation frequencies lying in sub-terahertz or terahertz (THz) bands, which makes them suitable for many practical applications. Amongst the other applications, AFM-based devices could be used for the creation of probabilistic logic with at least ten times higher operational frequencies than in existing devices based on ferromagnets. In this work we show a principle way of p-bit realization using AFM spin Hall oscillators (SHOs) operating in the regime of stochastic dynamics. We show numerically that the stochastic generation in an AFM-based SHO can be achieved for bias AC current magnitude and frequency varying in some ranges, and there are several regimes of stochastic SHO generation. Such a generating SHO can be utilized as a major element of easily-tuned p-bit operating at THz frequencies. We believe obtained results can be used for the research and development of AFM-based logic and high-operation-frequency calculation devices, paving an alternate approach for the solving of calculation-heavy classical problems like integer factorization.

ACKNOWLEDGMENTS

This work was supported in part by grant No. 22BF07-03 from the Ministry of Education and Science of Ukraine, grant 16F-2022 from the National Academy of Sciences of Ukraine, the NATO SPS.MYP G5792 grant, and the STCU grant 9918 (IEEE Magnetism in Ukraine Initiative).

Flexible Hair Tactile Array Based on Micro Magnetic Particles

Jiandong Man*, Jiamin Chen, Zhenhu Jin
Aerospace Information Research Institute, Chinese Academy of Sciences (China)
* manjiandong19@mails.ucas.ac.cn

Abstract ID #NMM-0500

Tactile sensing is an essential modality for humans to perceive the external environment. With the increasing popularity of household robots, precise grasping and safe human-machine interaction have become increasingly important. A crucial way to solve these problems is to endow robots with large-area tactile perception capabilities. In recent years, tactile sensors based on various principles have been developed. Among them, tactile sensors based on magnetic principles have the advantages of high resolution, low mechanical hysteresis, and non-contact measurement. In addition to film and convex structures, tactile sensors with hair structures have also been developed, which can greatly increase device sensitivity [1-2]. However, these studies often use a single hair or a small amount of hairs to achieve single-point measurement [3]. Therefore, it is difficult to apply them in robot skin or other fields requiring large-area perception, and it is also difficult to achieve complex functions. In this paper, we propose a magnetic hair array with tactile sensing ability. The array consists of 25×10 hairs, and the array area reaches 72 mm × 30 mm. Every hair in the array contains a large number of micro magnetic particles. When the external force acts on the hair array, multiple hairs will bend under the force. At this time, the size and direction of the stray magnetic field under the hair array will change. The magnitude and direction of the external force can be calculated by detecting this change through the magnetic sensor array under the hair array. The magnetic hair array is then applied to sliding tactile sensing and object recognition. It can realize precise detection of the size, direction, and sliding of external force and achieves a success rate of 97% in object recognition. In addition to recognizing the shape of objects, the magnetic hair array can identify whether the object has magnetism inside, which has great application potential in intelligent robots and rescue relief in the future.

ACKNOWLEDGMENTS

Research supported by the National Key R&D Program of China (2021YFB2011600), National Natural Science Foundation of China (Grant No. 61901440, 62271469), Beijing Municipal Natural Science Foundation (Grant No. 4202080), Young Elite Scientists Sponsorship Program by CAST (No. YESS20210341) and the One Hundred Person Project of the Chinese Academy of Sciences.

The authors thank the State Key Laboratory of Transducer Technology of Chinese Academy of Sciences for the help in the fabrication of this sensor.

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Local and Non-Local Effects in Curvilinear Micromagnetism

Oleksii Volkov*
Helmholtz-Zentrum Dresden-Rossendorf e.V. (Germany)
* o.volkov@hzdr.de

Abstract ID #NMM-0510

Dzyaloshinskii-Moriya interaction, also known as an antisymmetric exchange interaction, is the main source of chiral symmetry breaking effects in micromagnetic systems [1]. The later manifests itself in magnetic materials and layer stacks with structural space inversion symmetry breaking, where it leads to the formation of non-trivial chiral and topological spin textures (e.g. skyrmions, bubbles, homochiral spirals and domain walls). Such textures potentially could be utilized for prospective spintronic devices as a bit carrier. Still, tailoring of magnetochirality is only done by the selection of materials and adjustment of their composition in layer stacks.

Alternatively, we demonstrate that space inversion symmetry breaking of the magnetic order parameter appears in geometrically curved systems [2]. In curvilinear ferromagnets, curvature governs the appearance of geometry-induced chiral and anisotropic responses, which introduce a new toolbox to create artificial chiral nanostructures from achiral magnetic materials suitable for the stabilization of non-trivial chiral textures [2,3]. Moreover, curvilinear geometry also leads to the appearance of non-local chiral effects, that arise from the asymmetry of the top and bottom surfaces and existence of both in- and out-of-plane magnetization components of different parity with respect to the reflection procedure [4]. Recently, we demonstrate the existence of non-local chiral effects in geometrically curved asymmetric permalloy cap with the vortex texture [5]. We find that the equilibrium vortex core obtain both bend and curling deformation, that are dependent on the geometric symmetries and magnetic parameters.

ACKNOWLEDGMENTS

This work is done in collaboration with Denys Makarov, Oleksandr V. Pylypovskyi, Attila Kákay, Jürgen Fassbender (Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany), Daniel Wolf, Axel Lubk and Bernd Büchner (Institute for Solid State Research, IFW Dresden, Dresden, Germany) and Denis D. Sheka (Taras Shevchenko National University of Kyiv, Kyiv, Ukraine). This work is financed in part via the German Research Foundation (DFG) under Grants No. MA 5144/14-1, MA 5144/22-1, MA 5144/24-1, KA 5069/1-1, KA 5069/3-1, VO 2598/1-1 and MC 9/22-1.

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Unidirectional Spin-Wave Edge Modes in Magnonic Crystal

Michal Mruczkiewicz[1,*], Mateusz Zelent[2], Zhiwang Zhang[3], Johan Christensen[4], Tomas Scepka[1], Juraj Feilhauer[1]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Faculty of Physics, Adam Mickiewicz University in Poznan, Umultowska 85, Poznan, PL-61-614 (Poland)*

[3] *Department of Physics, MOE Key Laboratory of Modern Acoustics, Collaborative Innovation Center of Advanced Microstructures, Nanjing University (China)*

[4] *IMDEA Materials Institute, Calle Eric Kandel, 2, 28906, Getafe, Madrid (Spain)*

* michal.mruczkiewicz@savba.sk

Abstract ID #NMM-0529

The existence of topological edge states was demonstrated theoretically and experimentally in many wave-hosting systems, e.g. 2D electronic topological insulators or photonic, acoustic and mechanical metamaterials. Recently, several theoretical concepts predicted the existence of topological edge states in magnonic systems. Due to their robust transport properties, they are considered as a potential candidate for information carriers in future spintronic devices. However, the experimental demonstration of the magnonic topological edge states is still missing. The most significant challenges preventing the experimental observation of edge states include, e.g. complexity of the sample fabrication, control of the ground state or high density of modes in scaled-up system elements.

We present a numerical demonstration of magnonic crystal hosting unidirectional, topologically protected edge states [1]. The magnonic crystal is formed of dipolarly-coupled permalloy triangles. We show that due to the geometry of the unit cell, the size of the structure can be scaled up. In addition, the edge states can be found in a wide frequency range. Experimental detection of edge excitations in the considered system can be done with state-of-the-art techniques. Further, we demonstrate that the control of the magnonic crystal ground state can be realized by applying the external magnetic field locally. Therefore, we demonstrate a proof-of-concept of magnonic topological insulator nanostructure with simple geometry feasible for experimental realization.

A specific class of magnonic crystals hosting the unidirectional edge states is based on dipolarly coupled nanoelements with a unit cell magnetized in the closure domain state with fixed chirality [2]. The realization of the edge states relies there on the splitting of degeneracy of azimuthal modes under applied external magnetic field and was explained for isolated rings in terms of geometric Berry phase acquired by azimuthal spin wave [3, 4]. The unit cell of the magnonic crystal considered in our work is composed of a thin ferromagnetic square with two lines cut along its diagonals. Therefore the unit cell is consisting of four elementary building blocks, a right-angle isosceles triangles.

ACKNOWLEDGMENTS

The research has received funding from the Slovak Grant Agency APVV (grant number APVV-19-0311(RSWFA)), and VEGA agency, grant number VEGA-2/0177/21. This study was performed during the implementation of the project Building-up Centre for advanced materials application of the Slovak Academy of Sciences, ITMS project code 313021T081 supported by Research & Innovation Operational Programme funded by the ERDF (50%).

The research has received funding from National Science Centre of Poland, Grant No.~UMO-2018/30/Q/ST3/00416. The simulations were partially performed at the Poznan Supercomputing and Networking Center (Grant No. 398).

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Investigation of Self-Nucleation and Induction by Magnetic Moment of MFM Tip of the Skyrmion State Inside the Patterned Nanodots Multilayer Structure

Iuliia Vetrova[1,*], Mateusz Zelent[2], Ján Šoltýs[3], Tomas Scepka[1], Ján Dérer[1], Roman Stoklas[1], Vladimír Cambel[1], Michal Mruczkiewicz[4]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Faculty of Physics, Adam Mickiewicz University in Poznan, Umultowska 85, Poznan, PL-61-614 (Poland)*

[3] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava (Slovakia)*

[4] *Centre For Advanced Materials Application CEMEA, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava (Slovakia)*

* iuliia.vetrova@savba.sk

Abstract ID #NMM-0535

Magnetic skyrmions are circular domains surrounded by a single chirality domain wall [1]. They can be stabilized at room temperature by the Dzyaloshinskii-Moriya interaction (DMI) induced at the interface of the ferromagnetic/non-magnetic metals [2]. Stabilization of skyrmions inside the dot structures could lead to the development of an advanced concept of memory device that combines ultra-high density and fast data transfer rate.

We have experimentally and numerically demonstrated the formation of skyrmions in nanopatterned dots composed of six repetitions of the interfacially asymmetric Pt/Co/Au multilayer. Numerical simulations show an evolution of magnetic states as a function of dot diameter and the general tendencies of the energy levels of these states. These results are qualitatively consistent with the states observed in the experiment.

Next, we demonstrate experimentally switching between multidomain state to single domain state by localized field induced by an MFM tip. The numerical simulations show the possible evolution of the multidomain state to a single-domain state. Induction of the skyrmions from the multidomain state was demonstrated by numerical simulations when the pinning centres were introduced at the boundary of the dot.

ACKNOWLEDGMENTS

The work was supported by Slovak Grant Agency VEGA (Project No. 2/0168/22) and by the ITMS (Project No. 313021T081) supported by Research & Innovation Operational Programme funded by the ERDF.

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Optically Controllable Magnonic Crystal Based on Ferrit-Semiconductor Bilayer

Konstantin Bublikov[1,*], Milan Tapajna[1], Sergei Krylov[2], Dagmar Gregušová[1], Michal Kučera[1], Filip Gucmann[1], Michal Mruczkiewicz[3]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences. 841 04 Dubravska cesta 9, Bratislava (Slovakia)*
[2] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*
[3] *Centre For Advanced Materials Application CEMEA, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava (Slovakia)*

* elekbubl@savba.sk

Abstract ID #NMM-0537

Yttrium iron garnet (YIG) is an insulator magnetic material that is one of the most perspective materials for magnonics applications as having the lowest damping among the currently known ferrimagnets [1]. The recent progress in the direction of growing ultrathin yttrium iron garnet (YIG) layers atop the semiconductor substrates opens a new research direction: semiconductor magnonics [2]. Semiconductor magnonics is promising, e.g., for the integration of magnonic elements into classical microelectronics, and offers new methods of control over the spin wave spectra [2,3].

In this work, we study the microwave properties of YIG - gallium arsenide (GaAs) interface in order to apply it to designing the magnonic crystal (MC) with external optical control. MC are the magnonics waveguide structures with artificially created periodicity. Periodic lattice leads to the formation of the magnonic gaps in the spectra of propagation spin waves (SW) and MC are supposed to be widely used in magnonics for signal processing [4]. Potentially, the combination of YIG-GaAs bilayer and optical control will allow, e.g., to induce and reconfigure the MC lattice, and manipulate over magnonic band gaps opening and their frequency position [2,3].

We fabricated micro-scale MC composed of periodically grooved GaAs placed atop of planar stripe-shaped waveguide formed from the epitaxially grown YIG film. The GaAs sample was investigated by the Ohmic contacts resistance measurement under the laser irradiation exposure in order to obtain the dependence of charge carriers concentration vs the light intensity. We measured spectral characteristics of the SW transport through the fabricated structure versus the different power of the laser irradiation exposure. The electrodynamic simulations based on the finite element method were used to find the SW eigenwave solutions that belong to the YIG-GaAs bilayer. It allowed to relate the light-induced modification of SW spectra in the fabricated structure with the screening of the SW electromagnetic field by the light-induced charge carriers in the semiconductor.

At the conclusion of this research, we claim the possibility of the optical means control over the YIG-GaAs MC properties. In particular, it is possible to form and switch-off the magnonic gap and tune its frequency position. The obtained results will help, e.g., to design the smaller scales MC and MC with the periodic lattice induced by the optical patterns.

ACKNOWLEDGMENTS

The research has received funding from the Slovak Grant Agency APVV (Nos APVV-19-0311(RSWFA), and APVV-21-0365), and from VEGA (Project No. 2/0068/21). Furthermore, this study was performed during the implementation of the project Building-up Centre for advanced materials application of the Slovak Academy of Sciences, ITMS project code 313021T081 supported by Research & Innovation Operational Programme funded by the ERDF (15%).

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Nutation Modes in the Gyrotropic Vortex Dynamics in Circular Magnetic Nanodots

Kostyantyn Gusliyenko*
University of the Basque Country, UPV/EHU, San Sebastian and Ikerbasque, Bilbao (Spain)
* kostyantyn.gusliyenko@ehu.eus

Abstract ID #NMM-0539

A significant activity is devoted nowadays to the investigation of the ultrafast spin dynamic processes, holding a great potential for science and applications. However, a challenge of the understanding of the mechanisms of underlying spin dynamics in nanomaterials at pico- and femtosecond timescales remains under discussion [1].

In this talk, I report on the gyrotropic vortex dynamics in a circular magnetic nanodot, highlighting the impacts given by nutations [1] in the high-frequency part of the dot spin excitation spectrum [2]. The high-frequency vortex excitations in the framework of the nutation approach to the inertial dynamics in ferromagnets were considered. Based on the Thiele equation with a nutation term, we calculated the resonant frequencies and the dynamic susceptibility of a single vortex state in a magnetically soft nanodot excited by an in-plane oscillating magnetic field with a circular polarization. We showed the existence of two resonant mode frequencies reflected in two peaks of the dynamic magnetic susceptibility, corresponding to the vortex core gyrotropic motion and the nutations. The first frequency is the standard gyrotropic frequency, the value of which belongs to the sub-GHz range; the second frequency is responsible for spin nutations manifested themselves in the THz frequency range. The magnitude of the nutation frequency and the intensity of the dynamic response depend on the timescales of the nutation effects; the longer the nutation time, the lower the nutation frequency and more pronounced the response signal.

A distinctive feature of the considered vortex oscillations is the difference in the directions of spin rotation. Vortex core in the gyrotropic and nutation modes rotates in opposite directions. The resulting trajectory of the vortex core represents a superposition of precessional and nutational motions. Therefore, the vortex trajectory in a nanodot is affected by the nutations [2]. The nutation term in the initial Landau-Lifshits equation of magnetization motion leads to the appearance of a finite vortex inertial mass in the particle-like equation of motion of the vortex core. Our estimations showed that the magnitude of nutation-induced vortex mass depends on the nutation time, the sizes of nanodot, and the parameters of magnetic material; for the thin permalloy nanodot (with the radius of 100 nm, and thickness of 10 nm), it attains a magnitude of about g. Despite the rather small values of the nutation mass, even in comparison with the mass that arises due to the interaction of the spin waves with the moving vortex, taking into account its effect is important for the inertial dynamics of magnetization.

ACKNOWLEDGMENTS

I acknowledge support by IKERBASQUE (the Basque Foundation for Science). The research was supported by the Spanish Ministry of Science and Innovation grant PID2019-108075RB-C33 /AEI/10.13039/501100011033.

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Sub-terahertz Frequency Signal Source Based on an Array of Antiferromagnetic Tunnel Junctions

Oleh Shtanko*, Oleksandr V Prokopenko
Taras Shevchenko National University of Kyiv (Ukraine)
* olegshtanko2000@gmail.com

Abstract ID #NMM-0543

It has been shown recently [1] that an antiferromagnetic tunnel junction (ATJ) embedded in a high-Q dielectric resonator can operate as a sub-terahertz-frequency (STF) AC signal source having AC power exceeding that of 1 μW. Although the benefits of ATJs as core generating elements were analyzed in [1, 2] the proposed sources have one critical bottleneck: they are based on one junction only and thus have output AC powers less than 1–10 μW, which can be insufficient for some applications. To overcome this limit, in this paper, we consider an array of several independent ATJs placed at some "optimum places" inside the resonator, which could provide a substantial increase in the power generated by the source.

Every ATJ in our model is considered as a layered Pt/AFM/MgO/Pt structure consisting of a bottom current-driven platinum (Pt) layer adjacent to a layer of an Ir0.2Mn0.8 AFM and separated by a dielectric MgO spacer from the top Pt layer. A DC electric current in the Pt layer excites the transverse spin current flowing into Ir0.2Mn0.8 due to the spin Hall effect and causes the STF rotation of magnetizations in the AFM layer. The energy of STF rotating magnetization is collected due to the resonant transfer of this energy to a particular mode of the high-Q dielectric resonator having the same STF frequency as the frequency of rotating magnetization.

Using a simple electrical model developed in [2] for the case of independent ATJs connected to the dielectric resonator, we derive a general expression for the output AC power PAC of the source based on independent ATJs placed inside a high-Q dielectric resonator. We found that the use of only three ATJs allows one to exceed the frequency-dependent source output power up to 1–20 μW for the 0.1–1 THz frequency range. The obtained results can be useful for the development and optimization of STF signal sources based on AFM spintronic nanostructures.

ACKNOWLEDGMENTS

This work was supported in part by grant No. 22BF07-03 from the Ministry of Education and Science of Ukraine, grant 16F-2022 from the National Academy of Sciences of Ukraine, the NATO SPS.MYP G5792 grant, and the STCU grant 9918 (IEEE Magnetism in Ukraine Initiative).

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Nanomagnetism and Strain Effects in Magnetoelectric Antiferromagnet Cr_2O_3

Oleksandr V. Pylypovskyi*
Helmholtz-Zentrum Dresden-Rossendorf e.V. (Germany)
* o.pylypovskyi@hzdr.de

Abstract ID #NMM-0551

Concepts of the future of spintronics are often based on antiferromagnetic materials because of their attraction for low-energy operating and high-speed devices. However, an absence of significant net magnetization also results in challenges for manipulation and readout of the magnetic state. In this respect, room-temperature magnetoelectric easy-axis Cr_2O_3 is of special interest [1].

In a single-crystal Cr_2O_3 domain wall is a metastable excitation, which can be induced by a magnetoelectric poling procedure and being pinned by specially designed surface defects [2]. In contrast, thin films usually have a granular structure with significant amount of crystal defects acting as pinning sites for domain walls. Concentration and structure of the defects can be controlled by the film fabrication procedure, keeping the net magnetoelectric effect present for the sample [3]. Furthermore, low-defect films grown at sapphire can be persistently strained [4]. An out-of-plane magnetic moment formed by one of antiferromagnetic sublattices at the c-plane of Cr_2O_3 provides a possibility for the Hall magnetometry detecting magnetization direction by the Hall resistance measured in Pt capping layer [5].

The Neel temperature of bulk Cr_2O_3 of 35°C is the strong limiting technological factor for practical applications. There are theoretical and experimental demonstrations that the compressive strain induced by doping or procedure of growing at sapphire substrate leads to the substantial broadening of the antiferromagnetic phase by temperature increasing the Neel temperature above 100°C [4,6]. Furthermore, strained thin films can possess an inhomogeneous strain along the thickness, enabling net magnetization of flexomagnetic origin and vertical gradient of the Neel temperature. The latter provides a local flexomagnetic response which is controlled by the direction of the antiferromagnetic order parameter and scales with the sample's temperature [4].

We anticipate that Cr_2O_3 provides a flexible material platform for the fundamental and applied physics by demonstration of unique crystal-symmetry-assisted effects.

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Observation and Study of Curie Temperature Shift in Ni_xPt_{1-X} Alloy

Branislav Stropkai*, Serhii Vorobiov, Erik Cizmar, Vitalii Latyshev, Vladimir Komanicky
Department of Condensed Matter Physics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, 041 54 Košice (Slovakia)
* branislav.stropkai@student.upjs.sk

Abstract ID #NMM-0555

Each magnetically ordered material is characterized by its transition temperature. For ferromagnets, it is the Curie temperature. There are many ways to influence this characteristic, e.g. composition, annealing, pressure, grain size, etc.

Many of these influences are well documented and explained, yet it is most inspiring when a physical system defies an established model. Here we present an unexpected behaviour of a ferromagnetic alloy in which the Curie temperature strongly decreases when annealed.

This research has been motivated by the study of mesoscopic and nanoscopic wires of $Ni_{66}Pt_{34}$ alloy. In an attempt to improve magnetic properties of these wires, they have been annealed in temperatures over 700 K. After subsequent temperature dependent magnetic measurements, the Curie temperature was revealed to drop by 50 K in electrodeposited wires, and 25 K in sputtered samples. This is a highly unusual behaviour as annealing promotes the release of mechanical stress, grain growth and defect mobility, which are all processes resulting in the stabilization of domain walls and subsequent rise in curie temperature [1][2][3].

We have experimentally studied the possible mechanisms which might cause such a behaviour in a binary alloy. Our results restrict the array of possible phenomena causing this response and produce a better understanding of processes happening in these samples.

We believe these findings will set a stage for a more comprehensive study to provide an explanation of this behaviour. Understanding the mechanism of this phenomenon would provide a new possibility to tune properties of magnetic materials and expand upon the toolset available to material engineers.

ACKNOWLEDGMENTS

Work at Šafárik University has been supported by the grant of the Slovak Research and Development Agency under the contract No. APVV-20-0324.

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Module Trap for Magnetic Nanoparticles Concentration

Anatoliy Lapchuk[1], Alexander Prygun[1], Ivan Gorbov[1, 2,*], Dmytro Manko[1]
[1] *Institute for information recording, NAS of Ukraine (Ukraine)*
[2] *University of Nottingham (United Kingdom)*
* groznof@gmail.com

Abstract ID #NMM-0561

Nanoparticles are very promising for the investigation of biological objects at the molecular level and also in the early diagnosis and therapy of pathogenic processes [1, 2]. Magnetic nanoparticles (MNPs) can be easily and accurately manipulated at the nanoscale level and can be not harmful to living cells therefore can be used invivo analysis of cells [3].

MNPs can be used as vehicles for addressing drug delivery by their delivery and concentration at a required place by a strong gradient of magnetic force [4]. Magnetic nanoparticles with molecular traps for pathogen markers can be used to catch, transport, and concentrate the pathogen markers. The concentration of pathogen markers can be used for a strong increase in signal intensity and enhancement of the method of early detection. For many applications, it is also very important to have magnetic nanoparticles of definite size. Therefore, it is very important to have a magnetic system that can produce strong magnetic nanoparticle concentration and could provide a possibility of their separation by size. One of the possible ways to trap and sort nanoparticles under flow conditions is using a microfluidic device with an integrated flat micro-patterned hard magnetic film [5]. However, the described device can't concentrate all MNPs in a small area. Moreover, MNPs settle down directly to the magnetic film that needs further careful cleaning, at that the manufacture of such film is rather difficult.

We propose a module magnetic system for MNPs concentration. The system is based on several blocks of magnets with alternative orientations to produce strong gradient magnetic fields. The magnetic system is placed over the free surface of colloid running fluid with magnets without contact with liquid. MNPs are localized in fluid due to surface tension. Magnet system has contact with fluid only in the place where magnetic particles should be fixed or concentrated. The mathematical model of MNPs manipulation by the magnetic system and experiment setup are worked up. Mathematical simulation has proved that the magnetic system can provide a strong concentration of practically all magnetic nanoparticles in a small area. A mathematical simulation was confirmed by experimental measurement. It is also proved that the magnetic system provides the possibility of MNPs separation by size due to the different speeds of nanoparticles from bottom to surface in a gradient magnetic field. The module character of the magnetic system has a cumulative effect and allows easy change of system parameters. Since magnets have no direct contact with the colloidal liquid, the magnet system can be used many times without cleaning.

ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Ukraine (project No 2020.02/0090).

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Focused Ion Beam Influence on Topological and Magnetic Properties of the Nanostructures

Tetiana Kalmykova*, Sergei Krylov, Vladimír Cambel, Tomáš Ščepka
Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)
* tanya.kalmykova1@gmail.com

Abstract ID #NMM-0564

Today magnetism and magnetic nanostructures are of great interest. More and more studies are being conducted in topological magnonics[1], [2]. This area is associated with the study of spin waves in nanostructures. Studying this area in magnetism can make it possible to create magnetic storage devices with low energy consumption but high recording and storage density of information. However, exploring this area has challenges, primarily technological ones, such as complexity in the nanostructure manufacture, reproducibility, control of the relationship between structures, etc. [3]

The purpose of this work is to study the structures suitable for the implementation of uniaxial waves. To do this, we considered the influence of the Ga+ focused ion beam (FIB) on the magnetic properties of magnetic nanostructure from soft magnetic material (permalloy, Py). Such a structure is a square of different sizes, e.g., 400x400 nm, 800x800 nm, and 1.6x1.6 μm, cut into separate rectangles.

Preliminarily, with the help of numerical simulation in the mumax3 software [4], different properties of these structures were considered. These properties include the number and depth of the cuts, while their width was set to the constant value of 20 or 30 nm. In the next step, with the help of magnetic force microscopy (MFM) and scanning electron microscope (SEM), such structures were examined to confirm the simulation results. We have shown that removing (destroying) the exchange interaction between the elements is possible without reaching a complete physical separation of them. In this work, we provide a comparative analysis of the influence of the trenches' depth on the magnetic properties of the structure. Recommendations are given regarding doses of FIB necessary for switching from the initial "cross-like" state to single-domain; in the literature, it is often called "snake-like."

ACKNOWLEDGMENTS

We'd like to give a special thanks of gratitude to Ján Šoltýs, Ing., PhD. for providing aid in this research. We'd also like to thank Ján Fedor, Ing., PhD. for sample production.

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Nanostructures for Topological Magnonics

Sergei Krylov*, Tetiana Kalmykova, Vladimír Cambel, Tomáš Ščepka
Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)
* elekkryl@savba.sk

Abstract ID #NMM-0565

The current development of technologies in the field of nanomagnetism[1], [2] makes it possible to control and control magnetic domains in nanostructures. Such opportunities open the way to creating magnetic storage devices with better characteristics, such as fast duty cycle and low power consumption. Ferromagnetic nanostructures with controlled magnetic domains are also very promising in areas such as electromagnetic radiation generation, topological magnonics, etc. Naturally, these studies face challenges, primarily technological ones, such as complexity in the nanostructure manufacture, reproducibility, control of the relationship between structures, etc. [3]

In this work, we expand our study of the magnetic structures suitable for implementing uniaxial waves [4]. We used squares of different sizes from soft magnetic material (permalloy, Py). The Ga+ focused ion beam (FIB) separated each element into several parts. To perform our study, we started with the modeling in mumax3 software [5]. Then the theoretical results we got in the first step were experimentally confirmed using a magnetic force microscope (MFM) and scanning electron microscope (SEM). Close attention was paid to technological parameters that affect the magnetic properties of the sample under study. Such parameters include various widths of the cuts, which was not done in our previous study. It was also shown that adding a Ti buffer layer solves many issues related to the redistribution of atoms and significantly improves the precision and quality of the structure we study. Recommendations are also given regarding doses of FIB necessary for switching from the initial "cross-like" state to single-domain; in the literature, it is often called "snake-like.

ACKNOWLEDGMENTS

We'd like to give a special thanks of gratitude to Ján Šoltýs, Ing., PhD. for providing aid in this research. We'd also like to thank Ján Fedor, Ing., PhD. for sample production.

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Dynamics of Paramagnetic Centers in Organometallic Nanosystems and Their Application in Biomedical Research

Olena Aksimentyeva*, Yuliia Horbenko
Ivan Franko National University of Lviv (Ukraine)
* aksimen@ukr.net

Abstract ID #NMM-0582

A uniform magnetic field easy penetrates the body and does not change much inside it. Therefore, localizing a magnetic particle (magnetic or paramagnetic probe) and measuring any properties inside the body using magnetic measurement methods is easier. Until recently, radicals containing (• N = O) were used as a paramagnetic probe in medicine, which is very harmful to the body. On the other hand, during the oxidation-reduction processes in the living cell, free radicals form as intermediate products of biochemical reactions [1]. Ions of 3dn metals of the VIII group are known as the main source of free radicals causing the destruction of neurons. The basic idea of this work is to simulate a paramagnetic center surrounded by an organic matrix and to study the regularities of the EPR spectra transformation of this magnetic center at different temperatures.

We have studied the temperature transformations of the magnetic centers on model organometallic nanosystems – metalloorganic complexes and conjugated polyarenes doped with magnetic nanoclusters. Investigation of the magnetic center dynamics was carried out on powder samples, sealed in quartz ampules, using the EPR spectrometer of the X-ray range in the temperature interval of 4.2-300 K.

The shape of the EPR spectrum depends on the doping of the organic matrix by magnetic nanoparticles. Only one singlet line is observed at room and low temperatures for undoped samples of polyaniline, poly(ortho-anisidine), and poly(aminothiazole). This singlet without fine structure is caused by strong spin-spin interaction in a conjugated system. As a result of doping, two or three lines are observed with g-value from 2 to 4, confirming the formation of new paramagnetic centers in doped polymers.

A temperature dynamic of the EPR spectrum in doped polyarenes shows that a line width for the first resonance line increases for doped polymer and decreases for non-doped. At low temperatures in EPR spectra, a new line with g-value near 4 appeared. The EPR spectrum of poly(ortho-anisidine) doped with magnetic nanoclusters consists of two lines - low-temperature and high-temperature. Redistribution of the line intensity takes place with the temperature change. By quantum-chemical calculation of the structure of organometallic polymer complex, it has been revealed the presence of structural non-equivalence of its positions in conjugated polymer matrices [2]. The magnetic center behavior in metal-organic complexes of iron-1-nitrozo-2-naphtole [3] also demonstrates a redistribution of the intensity in the EPR spectrum with temperature changes.

So, the magnetic ion can act as a paramagnetic probe in its polymer complexes. It exhibits its own temperature behavior, different from the polymer matrix, and preserves it in a similar molecular environment. This phenomenon can be used in biology and medicine to monitor nerve cells.

ACKNOWLEDGMENTS

This work was partly supported by the Simons Foundation (Award Number: 1037973).

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Magnetic Properties of Two-Dimensional 1T-NiI_2

Juraj Mnich[1,*], Martin Gmitra[1,2]
[1] *Institute of Physics, Pavol Jozef Šafárik University in Košice (Slovakia)*
[2] *Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)*
* juraj.mnich@student.upjs.sk

Abstract ID #NMM-0589

Magnetic structure in multiferroic dihalides is affected by common geometrical frustration due to antiferromagnetic exchange interactions. One of the members of dihalid's family is NiI_2 which exhibits helical magnetic state. [1,2] Because of present space-inversion symmetry in 1T-NiI_2 the origin of helical states cannot be associated with Dzyaloshinskii–Moriya interaction. The true origin appears to be the consequence of strong magnetic frustration caused by an interplay of ferromagnetic and antiferromagentic exchange interraction in hexagonal lattices. [3] There is a problem in estimation of correct size of primitive magnetic supercell and also in appropriate helimagnetic state, which diverse from proper screw helix to in-plane cycloid. [4,5] Here we show that groundstate is the proper screw helix state associated with smaller magnetic unit cell. Instead of the 7x1 supercell we have found, using the first principles approach, that the 6x1 supercell is more favourable to describe groundstate of the 1T-NiI_2 monolayer with proper screw helix of magnetic moments. The sizes of supercells are expressed in units of former nonmagnetic unit cell. The formation of the proper screw helix breaks a symmetry of system and induces an electric polarization. Our results show the connection between the electric polarization and the direction of the proper screw helix. By applying an in-plane electric field one can induce a change in the polarization that drags also a change in the helical state leading to electrically induced switching of the helix state. The possibility to adjust magnetization using the electric field could provide various interesting applications of charge interconversion in spintronics.

ACKNOWLEDGMENTS

This work was supported by Slovak Research and Development Agency provided under Contract No. APVV-SK-CZ-RD-21-0114 and by the Ministry of Education, Science, Research and Sport of the Slovak Republic provided under Grant No. VEGA 1/0105/20 and Slovak Academy of Sciences project IMPULZ IM-2021-42 and project FLAG ERA JTC 2021 2DSOTECH.

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Thermally-Stable Subterahertz Frequency Spectrum Analyzer Based on an Array of Antiferromagnetic Tunnel Junctions

Volodymyr Prokopenko*, Oleksandr V Prokopenko
Taras Shevchenko National University of Kyiv (Ukraine)
* v.o.prokopenko@gmail.com

Abstract ID #NMM-0591

Antiferromagnetic spintronics is one of the emerging and promising fields of modern electronics suitable for the development and creation of micro- and nano-scale subterahertz frequency (STF) signal sources and detectors [1-3], which can be utilized in medicine, communications, security systems, etc. Each of these devices can be based on an antiferromagnetic tunnel junction (ATJ), which is a four-layer Pt/Antiferromagnet/MgO/Pt nanostructure compatible with the existing nanotechnology.

Theoretical models of STF signal sources and detectors based on ATJs were proposed in [1, 2]. Also, the noise properties of ATJ-based signal detector in the presence of Johnson-Nyquist thermal noise has been analyzed in a recent paper [3]. In this paper, we expand the formalism introduced in [3] and make a theoretical proposal of a thermally-stable STF spectrum analyzer based on several independent Pt/Ir0,2Mn0,8/MgO/Pt ATJs, which could be useful for signal spectrum analysis in a wide range of temperatures (~ 4 – 300 K).

We show that any ATJ depending on its geometrical and electrical parameters has some intrinsic frequency f corresponding to the "thermal insensibility" work point of the detector. At that frequency f output DC voltage of the detector does not depend on the detector temperature, which can be used for a more precise measurement of input STF signal power (without the account of thermal variations of detector parameters at the selected frequency f). We propose to use such a thermally-stable regime of an ATJ-based detector for the development of a thermally-stable STF spectrum analyzer, where an input signal is applied to a set of independent detectors having different intrinsic frequencies fi. Then by measuring the output DC signals of the detectors one can measure the signal powers at these frequencies fi with only minimal influence of temperature on the device performance.

The obtained results could be useful for the development and optimization of STF signal detectors and spectrum analyzers based on antiferromagnetic spintronic nanostructures.

ACKNOWLEDGMENTS

This work was supported in part by grant No. 22BF07-03 from the Ministry of Education and Science of Ukraine, grant 16F-2022 from the National Academy of Sciences of Ukraine, the NATO SPS.MYP G5792 grant, and the STCU grant 9918 (IEEE Magnetism in Ukraine Initiative).

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Curvilinear Antiferromagnetic Spin Chains: Interplay Between Geometry and External Magnetic Field

Yelyzaveta Borysenko[1, *], Denis D. Sheka[1], Kostiantyn Yershov[2], Juergen Fassbender[3], Jeroen van den Brink[4], Denys Makarov[3], Oleksandr V. Pylypovskyi[3]

[1] *Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *IFW Dresden (Germany)*
[3] *Helmholtz-Zentrum Dresden-Rossendorf e.V. (Germany)*
[4] *IFW (Germany)*

* yelyzavetapichko@gmail.com

Abstract ID #NMM-0598

Antiferromagnetically ordered (AFM) spin chains arranged along space curves represent a useful playground to study various possibilities of altering the sample's magnetic response by its geometry modification. The influence of curvature (κ) and torsion (τ) is characterized by effective magnetic interactions, namely anisotropic and Dzyaloshinskii–Moriya-like, which originate from exchange, dipolar interaction and intrinsic anisotropy [1, 2]. The strength of these interactions depends on κ and τ, determining the ground state and spin dynamics of such systems [2, 3].

Here, we investigate theoretically the interplay between geometrical and magnetic field effects in intrinsically achiral anisotropic spin chains shaped as rings (constant κ, no torsion) and helices (constant κ, τ) exposed to uniform static and rotating magnetic fields. Exposed to static magnetic field, bulk AFMs possess a high-field spin-flop state, characterized by reorientation of the order parameter. In contrast to the spin-flop phase for the model of a bulk easy-axis AFM, in ring-shaped spin chains the spin-flop state comprises two topologically different ground states depending on κ. We attribute them to the influence of curvature-induced Dzyaloshinskii–Moriya interaction, as well as the spin-flop transition being of first or second order depending on the ring curvature and the presence of an intermediate canted state for large κ [4]. In the helix-shaped spin chain, a rotating magnetic field induces domain wall propagation with velocity, which is proportional to the field frequency. The relation between the external field and geometrical parameters determines two motion modes: oscillating one and rigid motion with a constant velocity. Curvature and torsion strongly influence domain wall velocity and stability conditions of the rigid motion mode.

The obtained results could be useful for the development and optimization of STF signal detectors and spectrum analyzers based on antiferromagnetic spintronic nanostructures.

ACKNOWLEDGMENTS

Y. B. and D. Sh. acknowledge the financial support by the program "Magnetism in Ukraine Initiative" (IEEE Magnetics Society and the Science and Technology Center of Ukraine, Project No. 9918).

This work is financed in part via the German Research Foundation (DFG) under the Grants MC 9/22–1, MA 5144/22-1, MA 5144/24-1, and UKRATOP-project (funded by the BMBF; Reference No. 01DK18002).

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Molten Salt Synthesis of Manganese Pyrochlores ($R_2Mn_2O_7$, R = Y, Ho-Lu) at Ambient Pressure

Dovydas Karoblis[1, *], Agne Kizalaite[2], Tomas Murauskas[1], Aleksej Zarkov[1], Aivaras Kareiva[1], Sarah Stoll[3]

[1]*Institute of Chemistry, Vilnius University, Naugarduko g. 24, LT-03225, Vilnius, Lithuania (Lithuania)*
[2]*Vilnius University (Lithuania)*
[3]*Department of Chemistry, Georgetown University, 37th and O Streets NW, Washington, D.C. 20057, United States (United States)*

* dovydas.karoblis@chgf.vu.lt

Abstract ID #NMM-0603

Pyrochlores are a large family of inorganic compounds with the general formula $A_2B_2O_7$, which are subject to geometric magnetic frustrations and exhibit large quantum mechanical spin fluctuations [1]. Over 15 tetravalent ions can reside in the B site, while the A site is mostly occupied by a rare-earth element. In nearly all cases, pyrochlores can be prepared in ambient pressure, with the exception of a few vanadium-containing pyrochlores, and all manganese pyrochlores. Manganese pyrochlores ($R_2Mn_2O_7$) are prepared by using high-temperature as well as high-pressure or oxygen flow [2,3]. Moreover, the lanthanide manganese oxides form various structures with different oxidation states, like orthorhombic or hexagonal $RMnO_3$ (Mn^{3+}), RMn_2O_5 (Mn^{3+}, Mn^{4+}), and $R_2Mn_2O_7$ (Mn^{4+}); therefore the selective synthesis and formation of different phases is of high importance.

In this study, we report, a simple, low-temperature, time and cost-effective synthesis method for the selective preparation of $R_2Mn_2O_7$ pyrochlores by molten salt method for R = Y, and Ho-Lu. Our proposed synthetic technique is that it does not require high pressure or oxygen flow, or other additional oxidants. Moreover, for the R = Y, we demonstrate the phase-selective synthesis of o-$YMnO_3$, h-$YMnO_3$, and $Y_2Mn_2O_7$ by simply varying reaction temperature and precursors to chloride ratio. Various characterization methods, like X-ray powder diffraction and vibrational spectroscopy, were used to determine phase control and purity. A combination of Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) was performed to study morphology. Magnetic susceptibility was used to determine the magnetic ordering and oxidation states.

ACKNOWLEDGMENTS

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 778070 – TransFerr – H2020-MSCA-RISE-2017. SLS acknowledges support from the National Science Foundation (CHE1904616).

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Curvilinear Antiferromagnetic Spin Chains: Interplay Between Geometry and External Magnetic Field

Marko Milivojević[1, *], Martin Gmitra[2, 3], Marcin Kurpas[4], Ivan Štich[1], Jaroslav Fabian[5]
[1] *Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia (Slovakia)*
[2] *Institute of Physics, Pavol Jozef Šafárik University in Košice (Slovakia)*
[3] *Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)*
[4] *Institute of Physics, University of Silesia in Katowice (Poland)*
[5] *Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany (Germany*

*marko.milivojevic@savba.sk

Abstract ID #NMM-0618

Van der Waals heterostructures offer the possibility to modify different properties of a desired material via the proximity effect. In the context of the spin-orbit proximity effect [1-2], transition-metal dichalcogenides with strong spin-orbit coupling can be considered the best choice to induce and control the spin-orbit coupling in a desired material. We demonstrate that the WSe_2-P-WSe_2 heterostructure can be used to induce and control the spin-orbit coupling in phosphorene via different stacking configurations of the top and bottom WSe_2 monolayer. Focusing on hole spin physics in phosphorene, we obtained very good agreement between the ab-initio calculations and the effective spin-orbit Hamiltonian model, enabling us to compare the obtained spin texture and the proximity-induced spin-orbit coupling strength with ferroelectric phosphorene-like materials.

ACKNOWLEDGMENTS

This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Programme SASPRO 2 COFUND Marie Sklodowska-Curie grant agreement No. 945478.

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Orientational Anisotropy of Magnetic Damping in Ta/$Co_{20}Fe_{60}B_{20}$/MgO Heterostructures

Bivas Rana[1,*], YoshiChika Otani[2]
[1] *Institute of Spintronics and Quantum Information, Faculty of Physics, Adam Mickiewicz University, Poznan (Poland)*
[2] *Institute for Solid State Physics, University of Tokyo, Kashiwa (Japan)*
* bivran@amu.edu.pl

Abstract ID #NMM-0633

Magnetic damping, one of the key parameters of magnetic materials, governs the performance of many spintronics devices. Magnetic damping can be controlled by spin-torques [1], electric field [2]; and by engineering electronic band structures at the Fermi level [3]. Being a tensor quantity it also depends on the orientation of magnetization, known as orientational anisotropy, originates from the anisotropy in spin-orbit coupling (SOC) [4] and/or density of states (DOS) [5] in the ferromagnetic layer (bulk) and at the interfaces (for heterostructures made of ultrathin films) [5]. Therefore, orientational anisotropy provides a great tool for tuning magnetic damping by changing the orientation of magnetization, which is quite appealing from the application point of view. However, a detailed study of the orientational anisotropy in CoFeB based heterostructures, one of the key magnetic materials for spintronic applications, and its correlation with magnetic anisotropies, if any, have not been investigated yet.

Here, we report orientational anisotropy of damping in substrate/Ta(10)/$Co_{20}Fe_{60}B_{20}$(t)/MgO(2)/Al_2O_3(10) heterostructures with varying $Co_{20}Fe_{60}B_{20}$ layer thickness (t = 1.6 to 2.2 nm) deposited on Si/SiO_2 and $LiNbO_3$ substrates. The damping parameters are extracted by performing ferromagnetic resonance measurements based on spin pumping and inverse spin Hall effect technique [2]. The studied multilayers possess both: perpendicular magnetic anisotropy (PMA) with interfacial origin and in-plane magnetic anisotropy (IMA) with bulk origin. We observe that the orientational anisotropy of damping is composed of four-fold (α_4) and two-fold (α_2) anisotropy terms. We find that the α_4 originates from extrinsic two-magnon scattering (TMS), as the uniform magnons are scattered from inhomogeneities or imperfections present at the CoFeB interfaces (primarily at Ta/CoFeB interface) and consequently converted into degenerate nonuniform magnons. The α_2, on the other hand, originates from the anisotropy in bulk SOC of $Co_{20}Fe_{60}B_{20}$ film and correlates with IMA. Surprisingly, when IMA is very small for $Co_{20}Fe_{60}B_{20}$ heterostructures with Si/SiO_2 substrates, it has too little influence on α_2 to be experimentally identified. However, as IMA increases for $Co_{20}Fe_{60}B_{20}$ heterostructures with $LiNbO_3$ substrates, it starts to influence α_2 and shows a direct correlation between each other. Our results not only demonstrate the presence of both (four-fold and two-fold) anisotropies in damping, but also clarify their origins. These results will help to design the orientational anisotropy in damping in future spintronics devices by engineering bulk and interfacial SOC strengths.

ACKNOWLEDGMENTS

BR acknowledges RIKEN Incentive Research Project (Grant no. FY2019); ID-UB project (Grant no. 038/04/NS/0037); and the NCN SONATA-16 project (Grant no. 2020/39/D/ST3/02378). The authors sincerely thank Dr. Katsuya Miura and Dr. Hiromasa Takahashi from Hitachi Ltd., Japan, for preparing the thin films for the study.

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Phase-resolved Optical Characterization of Spin Waves

Ondřej Wojewoda, Martin Hrtoň, Meena Dhankhar, Jakub Krčma, Kristyna Davidkova, Jan Klíma, Jakub Holobrádek, Filip Ligmajer, Tomáš Šikola, Michal Urbanek*
CEITEC BUT, Brno University of Technology (Czech Republic)

* michal.urbanek@ceitec.vutbr.cz

Abstract ID #NMM-0635

When the spin wave wavelengths approach the exchange length of the magnetic material or when the dimensions of the magnonic system are reduced, new phenomena such as spin unpinning condition [1] arises. Nowadays, the only possibility to image nanoscale spin waves is X-ray microscopy, requiring synchrotron radiation and making investigation of nanoscale-related phenomena very time- and resource-demanding [2]. In our approach we show that the phase of spin waves can be characterized optically with sub-diffraction resolution and nanometer precision by using Mie resonance-enhanced Brillouin light scattering [3] with array of nanoresonators. The spatial restriction of the subdiffractional regions allows the light to interact with the spin waves with much shorter wavelengths, than is the wavelength of free-space light. Our experiments show that it is possible to track spin-wave phase with spatial step of 70 nm and measure the spin-wave wavelength with precission down to few nanometers. We performed this experiment for multiple frequencies and retrieved dispersion relation in the broad range of wavenumbers (from 0 to 30 rad/μm).

ACKNOWLEDGMENTS

We gratefully acknowledge CzechNanoLab project LM2018110 for the financial support of the measurements and sample fabrication at CEITEC Nano Research Infrastructure.

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A New Method of Study of Microwave Magnon-Plasmon-Polaritons

Oleksii V Malyshev[1, *], Volodymyr Y Malyshev[2], Gennadii A Melkov[2], Oleksandr V Prokopenko[3]
[1] *Taras Shevchenko National University of Kyiv, Faculty of Radio Physics, Electronics and Computer Systems (Ukraine)*
[2] *Institute of High Technologies Taras Shevchenko National University of Kyiv (Ukraine)*
[3] *Taras Shevchenko National University of Kyiv (Ukraine)*
* ClonStop@gmail.com

Abstract ID #NMM-0656

It is known that plasmon-polaritons can be easily observed at optical frequencies and in the terahertz band [1]. And if the media has magnetic properties then the optical or terahertz-frequency magnon-plasmon-polaritons (MPPs) in that media can be also excited and utilized. In contrast to the mentioned conventional "quasi-optical" MPPs microwave MPPs are exotic quasiparticles, which existence has been predicted only recently [2]. While in "quasi-optical" MPP its eigenfrequency depends on the media plasma frequency, the eigenfrequency of microwave MPPs can vary in a wide range, because the MPPs are formed due to a forced and tunable interaction of the surface electromagnetic wave with conducting magnetic media. The physics of microwave MPPs have not been studied yet, which makes them an interesting object for theoretical and experimental research. Also, such quasiparticles can be promising for some applications in microwave communications, material science, etc.

The first experiments involving microwave MPPs were performed for the surface electromagnetic wave resonator (SEWR) placed in a standard rectangular waveguide [3]. For such a system the coupling between the SEWR and the waveguide influencing the properties of the excited MPPs can be altered by changing the placement of SEWR inside the waveguide. Although that technique works, it is inconvenient and technically complicated. In this paper, we propose a new method of study of microwave MPP properties, which is based on the placement of SEWR in a standard – below-cutoff waveguide junction.

According to the proposed method, the SEWR is placed in the below-cutoff part of the standard – below-cutoff waveguide junction. The coupling between the incident TE_{10} wave mode (propagating in a standard waveguide and exciting the MPPs in a SEWR) can be varied by changing the distance between the resonator and the waveguide intersection plane, which can be rather easily implemented.

Using the proposed method, we study the frequency shift of the SEWR eigenfrequency due to the formation of microwave MPPs. For the resonator having a length of 11,25 mm, width of 1,35 mm, and thickness of 0,4 mm operating in the X-band and made of FeNi alloy, we observe a frequency shift of 44 MHz at the bias dc magnetic field of 100 mT. The observed effect has the same order of magnitude as in the previous experiments [3]. The proposed method and obtained results can be useful for the experimental investigation of microwave MPPs properties and for the development of devices utilizing microwave MPPs.

ACKNOWLEDGMENTS

This work was supported in part by grant No. 22BF07-03 from the Ministry of Education and Science of Ukraine, grant 16F-2022 from the National Academy of Sciences of Ukraine, the NATO SPS.MYP G5792 grant, and the STCU grant 9918 (IEEE Magnetism in Ukraine Initiative).

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Antiferromagnetic Self-Localized Structures Driven By Spin Current

Roman Khymyn[1,*], Roman Ovcharov[1], Boris Ivanov[2], Johan Akerman[1]
[1] *University of Gothenburg (Sweden)*
[2] *Institute of Magnetism of NASU and MESU, Kyiv (Ukraine)*
* khiminr@gmail.com

Abstract ID #NMM-0657

Antiferromagnets (AFMs) raises the interest for future spintronic applications, thanks to their unique properties, such as no stray field and spin current driven high-frequency dynamics. We demonstrate theoretically and by micro-magnetic simulations that self-localized AFM spin structures [1], driven by spin current, show peculiar dynamics that can substantially enrich the scope of functionalities in spintronics devices. Particularly, we consider a way to create and manupilate a domain wall, Bloch line and pure dynamic magnetic soliton, known as a droplet.

We show that a DW in a bi-axial AFM with the easy-axis type of primary anisotropy and driven by a spin current [2] is a close analog of a long Josephson junction and the Bloch line is a close analog to the Josephson vortex, also known as a fluxon state. The dynamics of the Néel vector inside the DW is described by a the same sine-Gordon type of equation as a Josephson phase Φ [3].

When the polarization of the spin current is parallel to the easy axis of an AFM, such a Bloch line can be nucleated at the edge of the AFM film and propelled by a current with exceptionally high velocities, up to ~10 km/s for a typical AFM film. The maximum achievable velocity depends on the damping constant of the AFM and the value of anisotropy, which, in turn, defines the maximum critical current of a DW stability. The above BL motion creates an alternate spin current at the read-out spin-Hall electrode, which can be employed for the easy detection of the BL dynamics. In contrast with a conventional LJJ, a DW has additional degrees of freedom, namely the position of its center, which can be manipulated by a spin current with a perpendicular polarization, and the distribution of the current along a DW.

We also demonstrate that the application of a spin current, inflowing from the nano-contact (NC), adjunct to an extended AFM film, can excite a dynamic self-localized soliton [4], equivalent to the ferromagnetic droplet [5]. We consider a system, which consists of a thin extended AFM film and NC, which provides STT. The anisotropy of the AFM is of the easy-axis type with the second-order term, and the STT polarization is parallel to the easy axis. At a particular sign of the secondary anisotropy, we observe a stable soliton at the currents above the threshold. A noticeable gap between the frequency of the droplet and AFM resonance appears at the threshold, which is also a remarkable feature of the droplet in the ferromagnetic oscillators. With increasing current, the frequency of the soliton becomes non-monotonic. It decreases with the expansion of the droplet profile and the edge of the droplet can be expanded far beyond the NC area. At higher current, the frequency increases, the droplet loses its stability, and the area under the NC instead emits propagating spin waves. We also show that a small anisotropy, perpendicular to the easy axis, can provide robust AC readout of the droplet spin dynamics.

ACKNOWLEDGMENTS

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant TOPSPIN No 835068).

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Structural and Magnetic Transitions in Aged Shape Memory Cu-Al-Mn And Cu-Al-Mn-Fe Alloys

Lesya Demchenko[1, 2,*], Anatoliy Titenko[3], Anatolii Kravets[4], Yurii Troshchenkov[3], Rostyslav Ponochovny[1], Oleksii Titenko[1]

[1] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
[2] *Stockholm University, Department of Materials and Environmental Chemistry (Sweden)*
[3] *Institute of Magnetism of NAS of Ukraine and MES of Ukraine (Ukraine)*
[4] *Institute of Magnetism, NAS of Ukraine (Ukraine)*

* lesyademch@gmail.com

Abstract ID #NMM-0674

Shape memory alloys (SMAs) are classified as "intelligent" materials that make it possible to create fundamentally new technologies in various branches of mechanical, aerospace, energy-saving, instrumental, and medical engineering. The promising functional nanocomposites are aging SMAs with thermoelastic martensitic transformation (MT) and high mechanical characteristics, able to generate significant reactive stresses beyond the material yield strength, as well as large reversible deformations in shape memory effect and superelasticity under significant loads. Some of the Cu-Al-Mn and Cu-Al-Mn-Fe alloys can exhibit unusual magnetic properties depending on their heat treatment, in addition to their mechanical and functional properties.

In this system, ferromagnetic nanosized particles of Cu2MnAl are precipitated due to aging, which contributes to an increase in the thermoelasticity of alloys associated with a decrease in the width of the temperature hysteresis [1]. Depending on the size and location of nanoparticles, the alloys of this system can exhibit superparamagnetic [2], ferromagnetic and antiferromagnetic ordering, giant magnetoresistance, magnetocaloric and magnetoelastic effects. Magnetization and magnetic anisotropy in the case of nanoparticles can be significantly greater than that of a bulk sample, and the difference between the Curie temperature (Tc) reaches hundreds of degrees.

In work, a comparative analysis of the structural and magnetic behavior of Cu-Al-Mn and Cu-Al-Mn-Fe alloys depending on their heat treatment is carried out. The influence of low-temperature aging on the behavior of induced martensitic transformation was established. Kinetic features of inducing martensitic transformations were noted in the alloys with iron doping. The magnetic behavior of Cu-Al-Mn and Cu-Al-Mn-Fe alloys is significantly different from each other, which is a consequence of the formation of the ferromagnetic Cu_2AlMn phase during isothermal aging in ternary alloys and the transformation to a superparamagnetic state in contrast to the quaternary composition doped with iron, in which antiferromagnetic ordering can be dominated. Due to nanoparticle precipitation in the alloy matrix due to the spinodal decomposition of solid solutions, the elastic scattering fields appear in the phase depleted with Mn. Such precipitates create a significant cumulative effect on the character and characteristic temperature of thermoelastic MT, as well as on both mechanical and magnetic behavior. The doping with Fe contributes to non-monotonic changes in MT temperatures.

ACKNOWLEDGMENTS

This research was supported by the Swedish Foundation for Strategic Research (grant UKR22-0042).

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Investigation of Valence Band Dispersion in (Ga,Mn)(Bi,As) epitaxial nanolayers

Oksana Yastrubchak[1,*], Nataliia Tataryn[1], Tadeusz Wosinski[2], Janusz Sadowski[2], Maciej Sawicki[2], Volodymyr Romanyuk[1], Sergii Mamykin[1], Lukasz Gluba[3], Olga Kondratenko[1]

Taras Shevchenko National University of Kyiv (Ukraine)

[1] *V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 41, 03028, Kyiv, Ukraine (Ukraine)*

[2] *Institute of Physics Polish Academy of Sciences (Poland)*

[3] *Institute of Physics, Maria Curie-Sklodowska University in Lublin (Poland)*

* plazmonoki@gmail.com

Abstract ID #NMM-0675

Dilute ferromagnetic semiconductors (DFSs) represent a class of alloys that combine semiconductor properties with magnetism in a single material. Their magnetic properties arise from transition metal ions introduced into the semiconductor parent lattice. The unique property of DFS spintronic devices is their capability of generating spin-polarized currents. In addition to the formation of spin current, of interest to spintronics, it is expected that the band structure changes arising from the presence of different doping ions such as Bi in the (Ga,Mn)As matrix, will lead to further development of novel DFS device concepts. The GaAs-based ferromagnetic semiconductor alloy compounds containing Mn and Bi emerged as potential candidates for novel nanoelectronic and spintronic applications.

We investigated 100 nm thick (Ga,Mn)(Bi,As) and (Ga,Mn)As layers with 4% Mn and 0.3% Bi contents, grown on GaAs(001) substrates by low-temperature molecular-beam epitaxy (LT-MBE) at a substrate temperature of 230°C. After growth, the samples were annealed in air at 180°C for 80 hours. We also investigated similarly grown 150 nm thick GaAs and Ga(Bi,As) layers as reference ones.

The superconducting quantum interference device (SQUID) magnetometry is used for the investigation of the magnetic properties of the heterostructures. Photoreflectance (PR) measurements are used for the determination of the band gap (Eo) and spin-orbit split-off (Eso) band to conduction band optical transitions. Besides the PR technique, the samples have been investigated by the μRaman spectroscopy to confirm the p-type character of Mn-doped films by the observation of the Coupled Plasmon-LO Phonon Mode (CPPM). The in-situ UV Angle-Resolved Photoemission Spectroscopy (ARPES) is used for the band structure analysis of the epitaxial layers. The low-temperature optical-energy-gap measurements supported by complementary characterization, for a series of (Ga,Mn)As, Ga(Bi,As) and (Ga,Mn)(Bi,As) nanolayers show that the deep modification of the GaAs valence band caused by Mn incorporation occurs for an Mn content much lower than that supporting dilute ferromagnetic phase in the investigated nanofilms.

The modulation PR spectroscopy, SE, and ARPES results are consistent with the valence-band model of hole-mediated ferromagnetism in the layers. These materials combine the properties of (Ga,Mn)As and Ga(Bi,As) ternary compounds and offer the possibility of tailoring the band-gap structure to the requirements of novel device functionalities for future spintronic and photonic applications. With and without Bi, a highly dispersing band crosses the Fermi level for the ferromagnetic Mn-containing layers. Furthermore, the Bi-doping induces modification and a narrowing of the spin-orbit split-off band. This can be attributed to the large spin-orbit interaction of the heavy Bi atoms (Z=83).

ACKNOWLEDGMENTS

O.Y. and N.T. acknowledge financial support from the Polish Academy of Science and the U.S. National Academy of Sciences. This work was also sponsored by the 2022 U.S.-Ukraine Alternative Energy Research Competition RFP and the IEEE program "Magnetism for Ukraine 2022", supported by the IEEE Magnetic Society under the Science and Technology Center in Ukraine (STCU) framework.

Ferromagnetic Resonance Excited by Interfacial Microwave Electric Field: The Role of Current-induced Torques

Bivas Rana[1,*], Angshuman Deka[2], YoshiChika Otani[3], Yasuhiro Fukuma[4]
[1] *Institute of Spintronics and Quantum Information, Faculty of Physics, Adam Mickiewicz University, Poznan (Poland)*
[2] *School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana (United States)*
[3] *Institute for Solid State Physics, University of Tokyo, Kashiwa (Japan)*
[4] *Department of Physics and Information Technology, Kyushu Institute of Technology, Iizuka (Japan)*
* bivran@amu.edu.pl

Abstract ID #NMM-0676

Excitation of magnetization dynamics in magnetic materials, especially in ultrathin ferromagnetic films, is of utmost importance for developing various ultrafast spintronics devices. Recently, the excitation of magnetization dynamics, i.e., ferromagnetic resonance (FMR) via electric field-induced modulation of interfacial magnetic anisotropies, has received particular attention due to several advantages, including lower power consumption [1]. However, several additional torques, generated by unavoidable microwave current induced because of the capacitive nature of the junctions, may also contribute to the excitation of FMR apart from electric field-induced torques [2]. Therefore, it is quite essential to estimate the contribution of microwave current induced torques on the excitation of ferromagnetic resonance and compare with electric field-induced torques, especially, at higher microwave power, higher frequency and larger junction area.

Here, we study the ferromagnetic resonance (FMR) excited by interfacial microwave electric field and investigate the role of current-induced torques. The FMR signals are excited by applying microwave signal across the metal-oxide junction in Si-SiO_2/buffer-layer(10)/$Co_{20}Fe_{60}B_20$(2)/MgO(2)/Al_2O_3(10) heterostructures with Pt and Ta buffer layers. The magnetic heterostructures posses both: perpendicular magnetic anisotropy (PMA) and in-plane magnetic anisotropy (IMA), with interfacial origin [3]. The presence of IMA enables the excitation of FMR by voltage-controlled in-plane magnetic anisotropy (VC-IMA) for in-plane orientation of magnetization, even though the voltage-controlled perpendicular magnetic anisotropy (VC-PMA) torque becomes zero in this configuration [1, 4]. Analysis of the resonance line shape and angular dependent behavior of resonance amplitude revealed that apart from VC-IMA torque a significant contribution can also arise from spin-torques (damping-like and field-like) and Oersted field torques originating from the flow of microwave current through metal-oxide junction. Surprisingly, the spin-torques and Oersted field torques are found to significantly contribute to the FMR excitation compared to the VC-IMA torque contribution, even for a device with negligible junction current. Notably, the contribution from the spin-torques and Oersted field torques further increases in the presence of a small junction current in the device. Our study shows that utmost care should be taken while analyzing the VC-PMA, VC-IMA induced FMR excitation results. As a guideline, the line shape analysis and angular dependent behavior should always be performed to confirm the electric field-induced excitation. These results will be quite useful for designing all-electric field controlled future spintronic devices.

ACKNOWLEDGMENTS

BR acknowledges RIKEN Incentive Research Project (Grant no. FY2019) and the NCN SONATA-16 project (Grant no. 2020/39/D/ST3/02378). The authors sincerely thank Dr. Katsuya Miura and Dr. Hiromasa Takahashi from Hitachi Ltd., Japan, for preparing the thin films for the study.

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Tuning of the contributions of the magnetically hard and magnetically soft phases in W/SmCo/W films

Oksana Koplak*, Federico Maspero, Alejandro Plaza, Riccardo Bertacco
Politecnico di Milano (Italy)
* oksana.koplak@polimi.it

Abstract ID #NMM-0689

Due to the excellent magnetic properties of SmCo there is a new trend in the development of SmCo micro- and nanostructures compatible with Micro Electromechanical System (MEMS) [1]. In literature, many reports on single-phase films such as SmCo5, SmCo7, and Sm2Co17 were presented. However, the case of mixed-phase samples is much less investigated, even though this situation is often encountered in practice and the interaction between different phases could give rise to interesting magnetic properties. To predict the magnetic properties of SmCo thin films, it is thus important to understand how the phase composition can be controlled at the nanometer level.

It is known that thermal annealing in vacuum leads to an increase in the coercive field in permanent micromagnets more than 20 kOe [2]. In this work, we demonstrate the possibility of controlling the phase composition of W/SmCo/W films by thermal annealing. The SmCo films were deposited by RF sputtering on a Si wafer. Annealing was performed in vacuum furnace at temperatures of 600 -750 C range. Structural and chemical characterization such as SEM, EDX, XRD, MFM experiments were carried out. The contributions from the magnetically soft and magnetically hard phases to the total magnetization of the film were found. The decomposition of the hysteresis loops of the samples after annealing was established amorphous phase, SmCo5 grain phase, intergranular SmCo5 phase, Sm2Co17 phase. Atomic fractions of magnetic phases in annealed samples were extracted. The in-plane and out-of-plane aligned grains of correspondent SmCo5 and Sm2Co17 phases in zero field demonstrated angular dependencies of magnetization Mrem (θ). The coexistence of these phases is an unusual result of short thermal annealing. The approximation is well-matched with the experimental Mrem (θ) curve, showing a possibility of a grain-size selective manipulation of magnetization in the SmCo films, by adjustment of the field, which regulates the range of sizes for the grains, involved into the magnetization reversal process.

ACKNOWLEDGMENTS

This research is part of the EU project M&MEMS (https://mandmems.eu/).

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Switching of Ferromagnetic Nano-Triangles by MFM Tip

Tomáš Ščepka[1,*], Juraj Feilhauer[1], Jaroslav Tobik[2], Sergey Krylov[1], Tetiana Kalmykova[1], Michal Mruczkiewicz[3]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Institute of Electrical Engineering, Slovak Academy of Sciences (Slovakia)*

[3] *Centre For Advanced Materials Application CEMEA, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava (Slovakia)*

* scepka.tomas@gmail.com

Abstract ID #NMM-0691

Dipolarly coupled magnetic elements are in the focus of research due to their potential applications in magnetic devices. For instance, an array of coupled elements forming spin ice are considered for memory applications [1], reservoir computing [2], or computations [3]. Further, a reconfiguration magnonics is often relying on arrays of switchable coupled elements [4]. Here, we focus on the control of chirality of the closed domain state in a magnetic structure formed by four isosceles Py triangles.

We demonstrate that at a certain value of applied in-plane magnetic field, the magnetic force microscopy (MFM) tip can induce a transition between the onion state and the closed domain state of the patterned nano-elements. The closed domain state remains stable during the rest of the scan. Therefore, the chirality of the closed domain is dependent on the direction of the MFM scan, since only two of four triangles are switched during the scan. Our results show that the MFM tip can serve to control the chirality of the closed domain state formed by four isosceles Py triangles (square cut along diagonals). This geometry is advantageous from the point of view of fabrication (cutting only straight edges) and dipolar coupling between elements. The realization of the magnonic crystals based on such unit cell could host interesting dynamical effects, e.g., unidirectional spin waves.

ACKNOWLEDGMENTS

We kindly acknowledge support of this work by Slovak Grant Agency APVV, grant number APVV-19-0311(RSWFA) and to VEGA agency, grant number VEGA-2/0177/21 and VEGA-2/0168/22. We also acknowledge support from CEMEA, ITMS project code 3130217081.

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Spin Wave Analysis in Perpendicularly Magnetized Uitra Thin $Co_{20}Fe_{60}B_{40}$ Films

Sreedevi Janardhanan[1,*], Aleksandra Trzaskowska[1], Mathieu Moalic[1], Sławomir Mielcarek[1], Piotr Kuswik[2], Maciej Krawczyk[1]

[1] *ISQI, Faculty of Physics, Adam Mickiewicz University in Poznań, Poland (Poland)*
[2] *Institute of Molecular Physics, Polish Academy of Science, Poznań, Poland (Poland)*
* srejan@amu.edu.pl

Abstract ID #NMM-0692

Magnonics, is an emerging field of research and technology, has been established to meet with the requirements of future signal processing devices by application of spin waves (SWs), which can transfer a spin for large distance without charge transfer, what minimizes the energy cost of logic operations. This investigation shows the interaction between spin waves, based on CoFeB/Au multilayers with Perpendicular Magnetic Anisotropy (PMA). The composition exhibits small pumping effect, hence low damping together with PMA effect, will promising for future applications in magnonics. In ordered to quantify the magnon energy, here we implemented Brillouin Light Scattering (BLS) method. We observed Interfacial Dzyaloshinskii-Moriya Interaction (iDMI) and characterized the strength by means of DMI coefficients. The synergy of PMA and DMI can be considered as interesting thing here, due to their high magnetic energy in order to reduce the volume of magnetic storage media and necessities to make chiralities which effects the whole magnetic properties. Furthermore, here we emphasis field and thickness dependent studies by employing Ferromagnetic Resonance (FMR) and BLS methods. Spin wave dispersion relations were extracted and studied the nonlinear effect as well as system behaviour. Opposed to the conventional dispersion relations of magnetic multilayers, it shows anomalous characteristics [1-5].

ACKNOWLEDGMENTS

This work was supported by Polish National Science Centre under grant no. UMO - 2020/37/B/ST3/03936 and ID-UB Grant no: UMO - 054/13/SNŚ/0033.

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Influence of Paramagnetic GGG Substrate on YIG Films at Millikelvin Temperatures

Rostyslav Serha[1,*], Andrey Voronov[1], David Schmoll[1], Roman Verba[2], Sabri Koraltan[1], Kristyna Davidkova[3], Barbora Budinská[1], Qi Wang[4], Oleksandr Dobrovolskiy[1], Michal Urbanek[3], Morris Lindner[5], Timmy Reimann[5], Carsten Dubs[5], Claas Abert[1], Dieter Suess[1], Sebastian Knauer[1], Andrii Chumak[6]

[1] *Faculty of Physics, University of Vienna (Austria)*
[2] *Institute of Magnetism of NAS of Ukraine and MES of Ukraine (Ukraine)*
[3] *CEITEC BUT, Brno University of Technology (Czech Republic)*
[4] *Huazhong University of Science and Technology (China)*
[5] *Innovent e.V. Technologieentwicklung, Jena (Germany)*
[6] *University of Vienna, Faculty of Physics, Boltzmanngasse 5, A-1090 Vienna (Austria)*
* rostyslav.serha@univie.ac.at

Abstract ID #NMM-0700

Magnonics is the field of science that deals with data carried by spin waves and their quanta, magnons, in magnetically ordered media [1]. The ferrimagnet yttrium iron garnet (YIG) Y3Fe5O12 is the material with the lowest known magnetic damping [2] and therefore often used in experiments and RF technologies. The use of YIG films of thicknesses down to tens of nanometers grown on gadolinium gallium garnet (GGG) Gd3Ga5O12 substrates [2] enables the development of magnetic devices and circuits at the nanoscale [3]. Recently, the field of quantum magnonics, operating with single magnons and versatile hybrid structures at millikelvin temperatures, attracts significant attention [3-5]. However, it is known that lowering the temperature increases the magnetic damping of YIG, which is usually associated with the influence of the paramagnetic GGG substrate [6,7].

In this work, we present the experimental findings on the affect of GGG substrate magnetization on the spin dynamics in YIG. The measured sample was a 97 nm-thick YIG film grown on 500 μm-thick GGG substrate and cut into a quadratic chip with an edge length of 5 mm. We have performed stripline ferromagnetic resonance (FMR) spectroscopy up to 40 GHz, using a physical property measurement system (PPMS), operating at the temperatures between 2 K and 400 K and a dilution refrigerator capable of reaching temperatures of 10 mK. The magnetization of the GGG substrate was measured via vibrating-sample magnetometry in the PPMS. The Gd3+ ions in GGG have a spin S = 7/2 and its saturation magnetization is about Ms = 805 kA/m.

At millikelvin temperatures, the GGG can be saturated to a significantly high value of hundreds of kA/m when magnetic fields of several hundred millitesla are applied. The GGG magnetization results in the formation of a stray field in the YIG film that affects the magnetization dynamics within it. The highly inhomogeneous stray field is oriented in the opposite direction to the external field in the case of in-plane magnetization of YIG/GGG and shifts the FMR frequency to lower values. Moreover, the FMR linewidth ΔB, which is a measure of magnetic damping in the system, is increased by the magnetization of GGG by more than eight times compared to measurements at room temperature. On the one hand, the stray field induced by the GGG is very inhomogeneous over the area of the YIG film, which was shown by our numerical simulations of the stray field. On the other hand, the magnetic system of the YIG can couple to the now partially ordered spin system of the GGG, providing an additional dissipation channel for resonance excitation.

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Structural Evolution and Magnetic Properties of the Ni-Fe Nanocomposite Particles Synthesized by Annealed the Mixture of Metal Nitrates and Polyacrylonitriles

Chun-Rong Lin*, Ying-Zhen Chen, Pei-Ying Chuang, Li-Huai Huang, Zi-Hao Huang, Kun-Yauh Shih
National Pingtung University (Taiwan)
* crlinspin@gmail.com

Abstract ID #NMM-0701

Nickel-iron alloys are an interesting material presenting intriguing behaviour and have many functional applications. Among them, the Permalloy ($Ni_{80}Fe_{20}$) alloy is the most widely used magnetic materials because its' high permeability, zero magnetostriction, low coercivity, and good anticorrosion properties. In this work, a series of carbon-encapsulated nickel-iron compound nanocomposite particles (NCPs) were synthesized by heat treatments the precursor of Ni-Fe-complex at temperatures TA between 300 °C and 1000 °C in an argon gas. The precursor of Ni-Fe-complex were synthesized by dissolved polyacrylonitrile powder and metal nitrates in dimethylacetamide, and heated at 200 °C for 1 hour. The influence of the synthesis temperature on the emerging phases of nanocomposites was investigated by several methods, including X-ray diffraction (XRD), Thermogravimetric analysis (TGA), Raman spectroscopy and transmission electron microscopy (TEM). XRD pattern show that the nickel carbide (Ni_3C)-like hexagonal-close-packed (hcp) structural phase, Fe-doped Ni_3C nanoparticles, was detected for precursor heated at T_A =300 °C. It is suggested that the Fe-doped Ni_3C structural phase is formed as an intermediate phase during the thermal pyrolysis of Fe-doped Ni3C into face-centered cubic (fcc) Permalloy ($Ni_{80}Fe_{20}$) alloy and carbon. For the precursor heated at T_A between 400 °C and 800 °C, the XRD spectrum contains both fcc Ni-Fe peaks and additional peaks corresponding to another hcp phase. Moreover, the XRD spectrum is dominated by the fcc phase. For the sample heated to $T_A \geqslant$ 900 ° C, the XRD spectrum indicates that all diffraction patterns maybe fully indexed considering a single fcc structure. The mean crystallite size of the fcc phase in NCPs varied from 9.7 to 30.5 nm by changing the temperatures TA. Magnetic measurements show that the saturation magnetization (Ms) of samples increase with increasing both fcc phase content and mean crystallite size. Raman spectra indicated the encapsulated carbon shells around the NCPs have the G-band and D-band centered at about 1593 cm-1 and 1348 cm-1, respectively. The relative intensity ratios of the D- and G-bands (I_D/I_G) for NCPs decreases with the annealing temperatures increase and the D-bands display a red shift behaviour, which demonstrates that the degree of graphitization increased with the annealing temperature. To clarify the structural evolution that exist in the samples and their magnetic contributions, the electronic structure and micromagnetic structure of all samples are investigated by the X-ray photoelectron spectroscopy (XPS) and Mössbauer spectroscopy.

ACKNOWLEDGMENTS

We are indebted to the National Pingtung University, and National Science and Technology Council of Taiwan (NSTC 111-2112-M-153-003-, NSTC 111-2811-M-153-001, and NSTC 108-2923-M-153-001-MY3). (NSC95-2112-M-218-001) for the financial support of this work.

Influence of Underlayer on Surface Acoustic Waves Velocity in CoFeB/MgO Heterostructure

Shashank Shekhar[1,*], Bivas Rana[1], Sławomir Mielcarek[2], Aleksandra Trzaskowska[2]
[1] *Institute of Spintronics and Quantum Information, Faculty of Physics, Adam Mickiewicz University, Poznan (Poland)*
[2] *ISQI, Faculty of Physics, Adam Mickiewicz University in Poznań, Poland (Poland)*
* shashank.shekhar@amu.edu.pl

Abstract ID #NMM-0707

Surface acoustic waves (SAWs), elastic waves propagating along the surface of an elastic material, can be used to estimate the elastic properties of the multilayers through the characterization of their dispersion relation (the relation between frequency and wavelength of the SAWs). In thin film-based multilayers, the properties of SAWs strongly depend on the elastic properties of the constituent layers as it affects the overall elastic stiffness of the multilayers. The magnetic thin film-based heterostructures possess intriguing magnetic and interfacial properties, which can control the static as well as dynamic properties of various spin textures, such as domain walls [1], skyrmions [2], and spin waves [3]. By coupling SAWs with those spin textures, it is possible to develop novel spintronics devices with improved performance and multiple functionalities. Therefore, understanding the SAW properties in magnetic thin film-based heterostructures like CoFeB/MgO, one of the most important [4,5] and promising candidates for spintronics applications, is very crucial as a first step.

In this study, we have shown the effect of mass loading (by varying the underlayer material) on the properties of SAWs (mainly Rayleigh waves) and hence the elastic parameters of the multilayers. We investigated Rayleigh-type SAWs in Si/SiO2(substrate)/X/Co20Fe60B20(1.4)/MgO(2)/Al2O3(10) multilayers employing the Brillouin light scattering (BLS) techniques, where X stands for Ta(10), W(10), Pt(10) and Ta(5)/Ru(20)/Ta(5). From the measured dispersion relations, we observed that the group velocities of SAWs decrease with increasing density ρ ($\rho Ta < \rho W < \rho Pt$), or overall mass (for Ta/Ru/Ta) of the underlayer material. We also performed numerical simulations based on the finite element method, which further supports our experimental results. Interestingly, the simulations, either considering the elastic parameters of individual layers or the elastic parameters of the uniform effective layer deposited on Si/SiO2 substrate, show the same results. Considering this observation, we further estimated the elastic properties of the uniform effective layer such as elastic tensor, Young's modulus, and Poisson's ratio and observed that the mass loading can efficiently modify the elastic parameters of the effective layer and thus the properties of SAWs. The estimated elastic parameters will be very helpful in further investigation of the coupling of SAWs with the spin degree of freedom (e.g., skyrmions, SWs, domain walls, magnetic vortices) in CoFeB/MgO heterostructure systems. Our study will not only contribute to the research field of SAWs (phononics) and spin waves (magnonics) but will also lead to a deeper understanding of the SAWs, spin waves and their coupling behavior in magnetic multilayer systems.

ACKNOWLEDGMENTS

SS would like to thank Adam Mickiewicz University for funding this project under IDUB (Grant no. 054/13/SNŚ/0031). BR acknowledges the NCN SONATA-16 project with grant number 2020/39/D/ST3/02378. All the authors sincerely thank Prof. YoshiChika Otani, Dr. Katsuya Miura, and Dr. Hiromasa Takahashi for providing thin films for the study.

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Propagating Spin-Wave Spectroscopy Studies in a Millekelvin Temperature Environment

David Schmoll[1,*], Sebastian Knauer[1], Rostyslav Serha[1], Roman Verba[2], Andrey Voronov[1], Carsten Dubs[3], Andrii Chumak[4]

[1] *Faculty of Physics, University of Vienna (Austria)*
[2] *Institute of Magnetism of NAS of Ukraine and MES of Ukraine (Ukraine)*
[3] *Innovent e.V. Technologieentwicklung, Jena (Germany)*
[4] *University of Vienna, Faculty of Physics, Boltzmanngasse 5, A-1090 Vienna (Austria)*
* david.schmoll@univie.ac.at

Abstract ID #NMM-0710

Technological advancements in the access to millikelvin temperatures, combined with high-frequency microwave technology, allow first steps towards the investigation of individual magnons in the field of quantum magnonics [1]. Such experiments require millikelvin base temperatures, to ensure a thermal magnon-free system [2]. We developed a cryogenic (down to 10 mK) propagating spin-wave spectroscopy setup, comprising a state-of-the-art dilution refrigerator, a 9-1-1 T vector magnet, and a 65 GHz-rated VNA measurement system. Spin-wave transmission was measured in a yttrium-iron-garnet (YIG) film on a 500 µm-thick gadolinium-gallium-garnet (GGG) substrate, using a microstrip antenna PCB. The obtained results were compared to room temperature measurements, performed with a standard electromagnet-based setup (see [3]), and revealed a decrease in the spin-wave frequency and an increase of the damping due to the paramagnetic GGG substrate. Spin-wave transmission is visible at temperatures down to 20 mK, with a shift to lower frequencies in spite the increased saturation magnetisation of YIG (see [4]). The influence of the paramagnetic GGG substrate on the damping was further investigated in temperature dependent Ferromagnetic Resonance (FMR) studies with a Physical Property Measurement System (PPMS) and the dilution refrigerator from 300 K down to 20 mK. The FMR results and complementary micromagnetic simulations reveal a qualitative connection between the spin-wave frequency shift and an increasing magnetic stray field of the paramagnetic GGG substrate. Considering the created magnetic stray field of GGG in a fit of the FMR-frequency with the Kittel formula, the decrease of the spin-wave frequency can also be confirmed quantitatively. The obtained results consolidate the understanding of spin waves at cryogenic temperatures and contribute to the emerging interest in the field of quantum magnonics. Furthermore, the demonstration of spin-wave propagation at cryogenic temperatures provides the technical capabilities and the environment for future investigations of individual magnons. Moreover, direct optical access to the dilution refrigerator, via optical fibres and small windows, allows millikelvin experiments in the field of hybrid opto-magnonic quantum systems.

ACKNOWLEDGMENTS

I would like to acknowledge the financial support of the Vienna Doctoral School of Physics.

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Ferromagnetic Resonance Study of Permalloy Nano-Rectangles

Pavol Neilinger[1,*], Tomáš Ščepka[2], Konstantin Bublikov[2], Ján Dérer[2], Miroslav Grajcar[1], Michal Mruczkiewicz[2]

[1] *Department of Experimental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*

[2] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

* pavol.neilinger@fmph.uniba.sk

Abstract ID #NMM-0711

Ferromagnetic resonance (FMR) is a sensitive technique to study the dynamical properties of magnetic ultrathin films and nanostructures. Here, we report on broadband ferromagnetic resonance study of an array of permalloy ($Ni_{80}Fe_{20}$) rectangles with side lengths 400 x 450 nm^2. The array of rectangles was patterned onto a 40 nm thick permalloy thin film using a lift-off process. The lattice constant of the rectangles was 1.6 μm and the entire field was 500x500 μm^2.

By use of the magnetic force microscopy (MFM) technique, we found that the magnetization states of the nano-rectangles of this sample had "S" and vortex magnetization states. FMR spectra were measured in the in-plane and out-of-plane orientation of DC bias magnetic field with respect to the plane of the arrays. Below 1GHz, the broadband ferromagnetic measurements are complemented with resonant measurements utilizing an RLC resonator. Based on the MFM image of the sample, we link the absorption in the FMR spectra to the different magnetization states of the nano-rectangles. Further, we performed time-domain simulations of the dynamic magnetization of a single rectangle in the initial magnetization in the "S" and vortex states, respectively. Then, the spectral density of the dynamic magnetization was obtained by fast Fourier transform (FFT). The obtained spectral densities are in qualitative agreement with the FMR absorption. Next, we analyzed the spatial dependencies of the FFT and obtained dynamic magnetization that corresponded to the spectral density resonance peaks. Comparing these data with the FMR measurements, we could determine the eigenmodes exited during measurements.

ACKNOWLEDGMENTS

We gratefully acknowledge financial support from the Slovak Grant Agency APVV, grant number APVV-19-0311 (SpinWave).

Non-reciprocal Magnonic Directional Coupler

Noura Zenbaa[1,*], Martin Gmitra[1,2]
[1] *Faculty of Physics, University of Vienna (Austria)*
[2] *Huazhong University of Science and Technology (China)*
* noura.zenbaa@univie.ac.at

Abstract ID #NMM-0713

Efforts in developing beyond CMOS technologies have been growing in recent years to overcome its limiting factors. Magnon-based computing, using spin waves as data carriers, has been proven to be a potential route to develop future alternative signal processing systems. A directional coupler serves as a universal building block in magnonic circuits and RF applications [1-3]. A magnonic directional coupler is realized by using two waveguides that are dipolarly coupled in a limited region where the energy of the wave excited in one waveguide can be fully transferred to the other after propagating over a certain distance, called the coupling length L. The dipolar coupling between the two waveguides leads to the splitting of the first width mode into two branches, corresponding to the symmetric and antisymmetric propagation of the spin wave. This coupling length L is defined as $\pi/\Delta k=\pi/|k_{as}-k_s|$, where k_{as} and k_s are the wavenumbers of antisymmetric and symmetric modes, respectively [1]. A magnonic half-adder based on two YIG nano-scale directional couplers has been demonstrated numerically and benchmarked [2].

In this work, we use a bilayer of YIG/CoFeB to construct the waveguides of the directional coupler to induce non-reciprocity in the spin-wave propagation and, therefore, add new functionalities to the directional coupler. The non-reciprocity due to the symmetry breaking leads to the splitting of Δk in one propagation direction being different compared to the other propagation direction ($\Delta k_+ \neq \Delta k_-$), in the Damon-Eschbach configuration. Therefore, the coupling length L will differ in the two propagation directions. At a special frequency, where $L_{-k} = 2L_{+k}$, the directional coupler can operate as a Y-circulator. The non-reciprocal spin-wave dispersion curves are numerically investigated in nm-thick bilayers of YIG(100)/CoFeB(40) and YIG(100)/SiO_2(5)/CoFeB(40) plane films as well as in nano-scale waveguides and measured using Ferromagnetic Resonance (FM) spectroscopy and k-resolved Brillouin Light Scattering (BLS) spectroscopy.

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Modification of Magnetic Semiconductors by Phosphorus Doping

Nataliia Tataryn[1,*], Oksana Yastrubchak[1], Sergii Mamykin[1], Volodymyr Romanyuk[1], Oleksandr Kolomys[1], Xinyu Liu[2], Jacek Furdyna[2], Badih A. Assaf[2], Olga Kondratenko[1]

[1] *V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 41, 03028, Kyiv, Ukraine (Ukraine)*

[2] *Department of Physics and Astronomy, University of Notre Dame, Notre Dame, IN 46556 USA (United States)*

* natalko1996@gmail.com

Abstract ID #NMM-0717

Dilute ferromagnetic semiconductors (DFMSs) represent a class of alloys that combine semiconductor properties with magnetism in a single material. Their magnetic properties arise from transition metal ions introduced into the semiconductor parent lattice. This combination of electronic and magnetic properties results in entirely new physical properties that are of interest in fundamental science and, importantly, hold the promise of a wide range of prototype devices relevant to the spintronics industry. Just as the introduction Mn in GaAs induces significant changes to the band structure of the parent compound, recent developments demonstrated that the band structure of the (Ga,Mn)As matrix itself can be further tuned by doping with In or Bi. In the quest for more efficient spintronic materials and a better understanding of topological effects in the band structure of (Ga,Mn)As, we study this band structure in on the quaternary (Ga,Mn)(P,As) compound.

Mn atoms substituting Ga in the GaAs host crystal, Mn_{Ga}, provide magnetism but also act as acceptors with an impurity binding energy of intermediate strength, 0.11 eV. This results in a large hole density, which is believed to play a crucial role in the hole-mediated ordering of Mn spins. On the other hand, Mn atoms occupying interstitial sites of the crystal lattice, MnI, act as double donors in GaAs and, together with the native As_{Ga} donors, partially compensate MnGa acceptors, thus resulting in effective reduction of the hole concentration in the (Ga,Mn)As films and, in turn, in decreasing their Curie temperature (T_C).

With P doping, strained (Ga,Mn)(P,As) films grown on GaAs, have been shown to host ferromagnetism with perpendicular magnetic anisotropy, ideal to observe the anomalous Hall effect. Mn and P co-doping also allow the tuning of the magnetic and electrical properties of this system independently.

Here, by combining Raman spectroscopy and optical ellipsometry, we are able to track the energy gap of (Ga,Mn)(P,As) at different levels of P doping, with and without Mn. Upon introduction of Mn, a strong couple of plasmon-phonon peak emerges in the Raman spectrum, along with an enhancement of the spectra absorption below the band edge. The shape of the band edge is consistent with a picture in which valence band dispersion near the edge is significantly altered, as in the impurity band picture.

Embedding P ions into the GaAs crystal lattice leads to an increase in the band gap, while Mn impurities lead to a decrease in it. A significant impact of Mn interstitial impurities on the structural and magnetic properties of the films was observed. We observe an enhancement of the charge density in the presence of Mn of the optical gap as well. The results suggest the presence of in-gap Mn impurity states and are not consistent with the observed blue shift of the Fermi level in (Ga,Mn)As, (In,Ga,Mn)As and (Ga,Mn)(Bi,As) epitaxial layers due to the Moss-Burstein effect.

ACKNOWLEDGMENTS

O.Y. and N.T. acknowledge financial support from Polish Academy of Science and U.S. National Academy of Sciences. This work was also sponsored by the CRDF 2022 U.S.-Ukraine Alternative Energy Research Competition grant (G-202206-68887) and the IEEE program "Magnetism for Ukraine 2022", supported by the IEEE Magnetic Society under the Science and Technology Center in Ukraine (STCU) framework. BAA, JF and XL also acknowledge support from NSF-DMR-1905277.

2D Bent Nano-Conduits Made of Partially-Compensated Ga:YIG for Spin-Wave Transport

Andrey Voronov[1,*], Ondřej Wojewoda[2], Kristyna Davidkova[2], Qi Wang[3], Carsten Dubs[4], Michal Urbanek[2], Andrii Chumak[5]

[1] *Faculty of Physics, University of Vienna (Austria)*
[2] *CEITEC BUT, Brno University of Technology (Czech Republic)*
[3] *Huazhong University of Science and Technology (China*
[4] *Innovent e.V. Technologieentwicklung, Jena (Germany)*
[5] *University of Vienna, Faculty of Physics, Boltzmanngasse 5, A-1090 Vienna (Austria)*
* andrey.voronov@univie.ac.at

Abstract ID #NMM-0719

The idea of using spin waves as data carriers in future computing devices has been developing over the years [1]. However, complex magnonic circuits require efficient guidance of spin waves between data processing and memory units in two dimensions. Even the simplest 90 degrees bend of a magnetic conduit is a challenge due to spin-wave anisotropy in the in-plane magnetised structures or the necessity of applying large magnetising fields in the out-of-plane geometry. Several solutions have already been proposed [2,3].

Here we investigate spin-wave transmission through a 90 degrees bent conduit made of partially compensated galium-doped yttrium iron garnet (Ga:YIG) in in-plane and out-of-plane magnetisation geometries. Ga:YIG opens access to operation with fast and isotropic exchange spin waves and has a pronounced uniaxial out-of-plane anisotropy leading to an out-of-plane easy axis [4]. The 500 nm wide and 69 nm thick Ga:YIG waveguide with 90 degrees curvature was fabricated using argon ion beam etching and positive CSAR 62 resist as a hard mask. Spin waves were excited by RF continuous or pulsed microwave signals applied to the CPW antenna and detected by space- and time-resolved micro-focused Brillouin light scattering (BLS) spectroscopy. The space-resolved investigation of the spin-wave intensity measured in the out-of-plane magnetisation geometry shows efficient spin-wave transmission through the curved region. The spin waves decay pattern after the bent region shows the oscillating behaviour associated with the interference between the higher spin-wave width modes [5]. The transmission efficiency is investigated as a function of the width of the nanowaveguide, the curvature of the bent, the magnetisation orientation as well as the spin-wave wavelength. The 2D Ga:YIG structures are great candidates for the implementation in complex magnonic circuits.

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Structural and Magnetic Properties of $Y_3Fe_5O_{12}$ Thin Films Grown on Metal Layers

Adam Krysztofik[1,*], Emerson Coy[2], Janusz Dubowik[3]
[1] *Faculty of Physics, Adam Mickiewicz University, ul. Uniwersytet Poznańskiego 2, 61-614 Poznań (Poland)*
[2] *NanoBioMedical Centre, Adam Mickiewicz University, ul. Wszechnicy Piastowskiej 3, 61-614 Poznan (Poland)*
[3] *Institute of Molecular Physics, Polish Academy of Science, Poznań, Poland (Poland)*
* adam.krysztofik@amu.edu.pl

Abstract ID #NMM-0726

We report on the structural and dynamic magnetic properties of yttrium iron garnet (YIG) films grown onto $Gd_3Ga_5O_{12}$ (GGG) [1] and $Y_3Al_5O_{12}$ substrates with thin platinum, iridium, and gold spacer layers. Separation of the YIG film from the substrate by a metal film strongly affects the crystalline structure of YIG and its magnetic damping. Despite the presence of structural defects, however, the YIG films exhibit a clear ferromagnetic resonance response. The ability to tune the magnetic damping without substantial changes to magnetization offers attractive prospects for the design of complex spin-wave conduits. We show that the insertion of a 1-nm-thick metal layer between YIG and GGG already increases the effective damping parameter enough to efficiently absorb spin waves. This bilayer structure can therefore be utilized for magnonic waveguide termination.

ACKNOWLEDGMENTS

A.K. acknowledges financial support from the National Science Centre Poland through the PRELUDIUM Project No. 2018/31/N/ST5/03433.

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Nonlinear Chiral Magnonic Resonators: Towards Magnonic Neural Networks

Kevin Fripp, Yat-Yin Au, Andrei Shytov, Volodymyr Kruglyak*
University of Exeter (United Kingdom)
* V.V.Kruglyak@exeter.ac.uk

Abstract ID #NMM-0743

We explore chiral magnonic resonators [1-5] as building blocks of artificial neural networks. Via micromagnetic simulations and analytical modelling, we demonstrate that the spin-wave modes confined in the resonators exhibit a strongly nonlinear response owing to energy concentration when resonantly excited by incoming spin waves. This effect may be harnessed to implement an artificial neuron in a network. Thereby, the confined and propagating spin-wave modes can serve as neurons and interneural connections, respectively. For modest excitation levels, the effect can be described in terms of a nonlinear shift of the resonant frequency ('detuning'), which results in amplitude-dependent transmission of monochromatic spin waves, which may be harnessed to recreate a "sigmoid-like" activation function. At even stronger excitation levels, the nonlinearity leads to bistability and hysteresis, akin to those occurring in nonlinear oscillators when the excitation strength exceeds a threshold set by the decay rate of the mode. In magnonic resonators, the latter includes both the Gilbert damping and the radiative decay due to the coupling with the medium. The results of our simulations are well described by a phenomenological model in which the nonlinear detuning of the confined mode is quadratic in its amplitude, while the propagation in the medium is linear.

ACKNOWLEDGMENTS

The research leading to these results has received funding from the UK Research and Innovation (UKRI) under the UK government's Horizon Europe funding guarantee (grant number 10039217) as part of the Horizon Europe (HORIZON-CL4-2021-DIGITAL-EMERGING-01) under grant agreement number 101070347, and from EPSRC of the UK (projects EP/L019876/1 and EP/T016574/1).

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Magnetic Helicoidal Dichroism in Resonant Scattering with XUV Light Vortices

Mauro Fanciulli[1,*], Matteo Pancaldi[2], Emanuele Pedersoli[3], Bernard Dieny[4], Giovanni De Ninno[2], Flavio Capotondi[3], Maurizio Sacchi[5, 6], Thierry Ruchon[7]

[1] *CYU Cergy Paris Université (France)*
[2] *Elettra synchrotron, Trieste, Italy (Italy)*
[3] *Elettra syncrhotron, Trieste, Italy (Italy*
[4] *SPINTEC, CEA Grenoble, France (France)*
[5] *INSP, CNRS - Sorbonne Université, Paris, France (France)*
[6] *Synchrotron SOLEIL (France)*
[7] *Attolab, CEA, Saclay, France (France)*

* mauro.fanciulli@u-cergy.fr

Abstract ID #NMM-0750

The polarization of a light beam is associated to the spin angular momentum (SAM) of the photon projected on its propagation axis, with $s_z=\pm1$ for circular and $s_z=0$ for linear polarization. A photon can carry also an orbital angular momentum (OAM), indexed by $\ell \in Z$, which corresponds in the wave picture to a helicoidal wavefront of light instead of a plane wave. The OAM of light, however, has been much less exploited than SAM as a probe in light-matter interaction.

We developed the classical electromagnetic theory for the reflection of light carrying OAM by a non-uniform magnetic material [1]. It is found that a beam of mode ℓ is modified into ℓ+n after reflection, where n identifies the symmetry properties of the magnetic structure seen by the beam in terms of azimuthal Fourier decomposition. This leads to a differential scattering that depends on the sign of ℓ, giving rise to what we called magnetic helicoidal dichroism (MHD) [1]. Different from magnetic circular dichroism (MCD), which is a local probe of the magnetic properties, MHD carries information about the overall topology of the magnetic structure.

I will present the first experimental observation of MHD measured at the FERMI free electron laser on a permalloy magnetic vortex at the Fe 3p resonance [2]. The experimental results agree with the theoretical predictions, setting the ground for scan-free investigations of ultrafast dynamics of magnetic structures with MHD, for which I will also show preliminary results.

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All-Optical Magnetic Switching of Ferromagnetic Nano-islands with a Low-power, Continuous-wave Laser

Holly Holder[1,*], Kilian Stenning[2], Xiaofei Xiao[1], Alex Vanstone[1], Jack Carter-Gartside[1], Oscar Kennedy[2], Rupert Oulton[1], Will Branford[1]

[1] *Imperial College London (United Kingdom)*
[2] *University College London (United Kingdom)*

* h.holder20@imperial.ac.uk

Abstract ID #NMM-0754

Nanomagnetic arrays offer new alternatives to current data storage technologies and computation. Competing interactions give rise to emergent behaviour, and have been shown to be capable of neuromorphic computing [1]. Accurate, precise control of the state of an individual nanomagnet will be crucial in accessing the full potential of these novel nanomagnetic systems. At present, local control relies on energetically costly heat-assisted technologies, while current AOMS schemes require large, ultrafast lasers, and exotic materials.

We have demonstrated complete and deterministic reversal of the magnetisation within individual Permalloy (Ni81Fe19, Ni50Fe50) nanomagnets, in the absence of an applied external magnetic field [2]. Magnetic switching is induced by a focused, continuous-wave, linearly-polarised, λ = 633nm laser spot moving across nanomagnets. Reversal is observed at low powers (as low as 2.74mW), with high switching fidelity across lines of illuminated nanomagnets, and individual nano-islands shown to repeatably, deterministically switch under identical illumination protocols.

Our results confirm the repeatability and robustness of this new and promising all-optical magnetic switching technique, with further work being undertaken to further elucidate the exact physical mechanisms underpinning magnetic reversal. The low cost and low powers of the lasers associated with this new approach would be ideal for future device integration.

ACKNOWLEDGMENTS

This work is supported by the EPSRC doctoral training partnership via Imperial College London. With thanks to: W. R. Branford, R. F. Oulton, K. D. Stenning, X. Xiao, J. C. Gartside, A. Vanstone, O. W. Kennedy.

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Magnetic Resonance Study of Disordered Nanoparticle Ensembles in Synthetic Diamond

Viktor Bratus[1,*], Bela Shanina[1], Igor Vorona[1], Valentyn Lysakovskyi[2], Sergii Ivakhnenko[2]
[1] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine (Ukraine)*
[2] *V. Bakul Institute for Superhard Materials, NAS of Ukraine (Ukraine)*
* victor.bratus@gmail.com

Abstract ID #NMM-0755

Synthetic diamonds have similar properties to natural ones making them indispensable in a variety of industrial applications and enabling step changes in process and end-product performance that are applicable to a wide array of industries including optics, quantum computation, semiconductors, and sensors. To achieve diamond synthesis in the laboratory, high pressure and high temperature conditions are needed. The production of synthetic diamond also requires the introduction of a metal catalyst into the reaction mixture. Being in the service as catalysts, alloys of the transition metals Fe, Ni, Co are involved into the final product as inclusions and nanoparticles. This presentation is focused on results of ferromagnetic resonance (FMR) and electron paramagnetic resonance (EPR) investigation of domestic synthetic diamonds.

Diamond single crystals were mainly grown in solution-melt systems based on Fe-Co doped with Ti, Zr and Mg or Fe-Ni catalysts. This makes it possible to obtain type Ib and type IIa diamond single crystals 5-15 carats in size with a controlled defect-impurity composition and growth rates. EPR and FMR measurements were performed in the X-band at room temperature.

Multifarious magnetic resonance spectra have been registered depending on type of metal catalysts and dopants. It has been found, that there are at least two distinct lines in low magnetic field belonging to FMR. The experimental spectra were simulated by a set of Lorentzian functions to find the angular dependence of the resonance fields for each signal and sample.

The theory developed for orientation of the magnetic moment of inclusions in the external magnetic field has allowed to describe the angular dependence of the resonance fields, when the magnetic field H is rotated in different planes. The magnetic characteristics of inclusions have been found from the fitting of the calculated angular dependence to the experimental data. For example, angular dependences for one kind of samples are related to the case when cubic axes of the FM particles are adjusted to cubic system of diamond. For other ones the angular dependences are very weak and not regular because two cubic systems are turned to each other.

In some cases, an unusual shape of the FMR spectrum has been attributed to superparamagnetism of ensemble of small magnetic nanoparticles.

ACKNOWLEDGMENTS

Support by the Institute of Electrical and Electronics Engineers (IEEE) Magnetics Society (Project No. 9918 "Magnetism for Ukraine 2022") is greatly appreciated.

Between Spin Waves and Magnetization Patterns: Spin Wave Freezing in Ferromagnetic Films with Dzyaloshinskii-Moriya Interaction

Pawel Gruszecki[1,*], Jan Kisielewski[2], Maciej Krawczyk[1], Vitalii Zablotskii[3], Andrzej Maziewski[2]
[1] *ISQI, Faculty of Physics, Adam Mickiewicz University in Poznań, Poland (Poland)*
[2] *Faculty of Physics, University of Bialystok, Bialystok (Poland)*
[3] *Institute of Physics, Czech Academy of Sciences, Prague (Czech Republic)*
* gruszecki@amu.edu.pl

Abstract ID #NMM-0760

Spin waves, the primary object of study in magnonics, are precessional perturbations of magnetization propagating in magnetic media. Recently, non-collinear magnetic textures have received increasing attention as media in which spin waves can propagate. However, the relationship between spin waves (propagating low-amplitude disturbances of magnetization) and magnetic textures (static and large-amplitude patterns of magnetization) is poorly understood. Here we investigate the relationship between spin waves in uniformly magnetized thin films and magnetic textures at remanence, focusing in particular on ultrathin films with perpendicular magnetic anisotropy and with Dzyaloshinskii-Moriya interactions (DMI) [1]. We focus our research on both systems, favoring stripe domain patterns [1] and spin spirals [2] as magnetization configurations in the absence of the bias magnetic field, and analyze spin wave dynamics in both uniformly and nonuniformly magnetized films. We show a close relationship between the softened spin-wave mode from the bottom of the spin-wave spectrum and the magnetization texture formed after the phase transition when the periodic magnetization texture emerges. Furthermore, we show that DMI nonreciprocity leads to the emergence of flowing magnetization patterns, suggesting a spontaneous breaking of translational symmetry and the formation of magnonic space-time crystals.

ACKNOWLEDGMENTS

We acknowledge the funding from the Polish National Science Centre (project No. UMO-2019/35/D/ST3/03729 and 2019/35/D/ST3/03729) and the Czech Ministry of Education, Youth, and Sports (project No. SOLID21–CZ.02.1.01/0.0/0.0/16_019/0000760).

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The Influence of the Magnetic Field on the Morphology and Structural Characteristics of Thin-Film Granular Magnetic Systems Co-Ag and Co-Cu as Functional Elements of Spintronics

Ihor Shpetnyy[1,*], Tomáš Plecenik[2], Yurii Shkurdoda[1], Iryna Nakonechna[1], Uliana Shvets[1]
[1] *Sumy State University, 2, Rimsky-Korsakov St., 40007 Sumy (Ukraine)*
[2] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava, Mlynska dolina F2, Bratislava 84248 (Slovakia)*
* i.shpetnyy@gmail.com

Abstract ID #NMM-0773

Granular magnetic systems based on Co-Ag and Co-Cu alloys have been used in spintronics [1], biotechnologies [2], medicine, and other fields due effects of giant and anisotropic magnetoresistance. Such structures are used to manufacture of elements of nonvolatile magnetoresistive memory, biosensors, sensors of the magnitude and the magnetic field direction. However, the design of such devices requires to take into account the effects of the magnetic field on the surface morphology of thin films and the impact of the magnetic aftereffect. When the spin current passes through thin magnetic films, a high-gradient magnetic field can arise due to the very small size of these elements. Such a magnetic field can affect the surface morphology and change the structural characteristics of the film. The effects of the influence of a magnetic field and magnetic aftereffect, which significantly change the structure and properties of nanomaterials, should be considered for design of nanoelectronics devices that running under the influence of magnetic fields. Even slight changes in the structure or morphology of the surface of the films can lead to device failures.

The effect of an external magnetic field on the mechanical and structural characteristics of the surface of samples of granular thin-film alloys based on Co and Ag, as well as Co and Cu, was studied using atomic force microscopy on a Solver PRO device. It has been established that even at a relatively low intensity (H = 0.01 T), the first application of a magnetic field has the most significant effect on the change in the sample surface morphology. So, for a sample of a granular alloy based on cobalt and silver at c_{Co} = 39 at.%, after the first application of a magnetic field, the arithmetic mean film surface roughness Ra decreased by 19%, the root mean square roughness Rq by 16%, and the structural entropy S by 4.5%. , and the height of the highest peak is 4 times. An increase in the magnetic field to H = 0.1 T and subsequent relaxation in the absence of a field had no significant effect on the structural characteristics of the film surface compared to the values obtained after the first application of an external magnetic field. The effects of a magnetic field on the structure and surface morphology of samples of granular film alloys can be explained by the rotation of magnetic granules, their deformation, and the transition of the film system to a new, more equilibrium state. This state differs in its properties from the initial one.

ACKNOWLEDGMENTS

This work was funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V01-00044 and Project № 9918 Magnetism in Ukraine Initiative.

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Aging Impact on Crystal Structure and Magnetic Parameters of $KFeO_2$ Nanoparticles

Olesya Nakonechna[1], Gurmeet Singh Lotey[2], Iryna Sharai[3,*], Andrii Bodnaruk[4], Victor Kalita[5], Alexandr Tovstolytkin[6]

[1] *Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *DAV University (India)*
[3] *Institute of Magnetism, NAS of Ukraine (Ukraine)*
[4] *Institute of Physics, NAS of Ukraine (Ukraine)*
[5] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
[6] *Institute of Magnetism of NAS of Ukraine and MES of Ukraine (Ukraine)*

* ira-sharay@ukr.net

Abstract ID #NMM-0791

The use of magnetic nanoparticles (MNPs) in medicine and biology has been extensively developed in last decades and has opened up new opportunities in the diagnosis of a number of diseases and their treatment [1, 2]. Magnetic hyperthermia therapy (MHT) is newly back in the interest of both, clinical and research oncologists, because of its properties to directly produce permanent damages of the treated tumors. Alkaline metal ferrite nanoparticles with the general formula $AFeO_2$ (where A = Li, Na, K, Ca) are considered as good mediators of MHT since they satisfy a number of basic requirements, namely: they are biocompatible, single domain, weakly agglomerated and demonstrate high heating efficiency under an alternating magnetic field [3]. However, the stability of nanoparticles remains an important problem since many factors may cause magnetic aging effect. Here, we report the aging impact on crystal structure parameters and main magnetic features of $KFeO_2$ nanoparticles.

As we have recently shown, the crystal structure of $NaFeO_2$ nanoparticles undergoes an essential change and leads to significant changes in magnetic properties with aging for 10,000 h [3]. Here, we provided the detailed XRD study of $KFeO_2$ nanoparticles subjected to a prolonged exposure (10,000 h) at room temperature (aging). The diffraction pattern of aged $KFeO_2$ sample generally reproduces the Fe_3O_4 diffraction spectrum and is indexed well in a cubic crystal lattice with lattice parameter a = 0.8337(2) nm, which is higher than that for as-prepared MNPs; the average coherent block size D increases essentially, while the lattice strain ε is reduced.

Magnetic properties were studied by the vibrating sample magnetometry at a temperature ranging from 300 to 500 K. It has shown that saturation magnetization becomes higher and Curie temperature tends to increase for the aged MNPs, but those characteristics remain almost unchangeable at magnetic hyperthermia-relevant temperatures (up to 315–320 K). We evaluated the heating capability of the aged and as-prepared $KFeO_2$ nanoparticles by varying the magnetic field strength and applied AC current frequency using COMSOL Multiphysics® software. The results of multiphysics simulation have revealed that the heating efficiency of as-prepared and aged $KFeO_2$ nanoparticles is temperature independent and keep a high magnitude, proving the wide perspectives in the use of nanoparticles studied in a biomedical applications.

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Enhencment of LTP Crystallographyc Phase in MnBi Alloy Systems

Tiberiu Roman[1, 2, 3,*], Marian Grigoras[3], Nicoleta Lupu[3]

[1] *"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, Carol I nr. 11 Blvd., Iasi 700506, Romania (Romania)*

[2] *Integrated Center of Environmental Science Studies in the North-Eastern Development Region (CERNESIM), Department of Exact and Natural Sciences, Institute of Interdisciplinary Research, Alexandru Ioan Cuza University of Iasi, 700506 Iasi, Romania (Romania)*

[3] *National Institute of Research and Development for Technical Physics, 47 Mangeron Boulevard, Iasi 700050, Romania (Romania)*

* tiberiu.roman@chem.uaic.ro

Abstract ID #NMM-0793

MnBi alloys represent an attractive alternative for replacing the rare-earth permanent magnets in different areas, especially at elevated temperatures. This alloy crystallizes either in a hexagonal P63/mmc space group type or in an orthorhombic Pmma space group type. The phases are temperature dependent during the processing stages and possess different magnetic behavior: the low temperature phase (LTP) is magnetically hard, while the high temperature phase(HTP) is magnetically soft [1]. A great challenge is to obtain a material consisting of pure LTP as this alloy is formed through a peritectic reaction between Mn and Bi. The resulting product consist most likely of MnBi in both crystallographic forms, unreacted Bi and Mn. In this work we will demonstrate that it is possible to obtain reproductible small amounts (g) of MnBi LTP with impurities bellow the XRD detection limit. For this purpose, we have developed a 2-stage separation process for the alloy batch which removes the unalloyed metals During the first stage, the Bi excess is eliminated through gravitational means using a system of quartz tubes, while in the second stage, the Mn excess is taken away during the ribbons formation through the melt spinning technique [2]. A content of over 99 wt.% LTP phase is observed in the 290°C thermally treated ribbons, while the saturation magnetization (MS) values reach 70.6 Am^2/kg at room temperature, for a maximum applied field of 0.9 T. We anticipate that different morphological forms of the alloy (e.g., powders or pellets of MnBi LTP) are strongly influencing the magnetic behavior because of different magnetic anisotropies. Small additions of Al, Cu or Co is influencing also the magnetic properties, once the LTP crystallographic phase is maintained within reasonable limits.

ACKNOWLEDGMENTS

Financial support from the NUCLEU Programme - Contract No. 18N/01.01.2023, project PN 23 11 01 01 is highly acknowledged.

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Chiral Domain Walls in Cylindrical Nanowires

José A. Fernandez-Roldan*
Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany. (Germany)
* j.fernandez-roldan@hzdr.de

Abstract ID #NMM-0796

In recent years, chiral domain walls in cylindrical nanowires, such as the Bloch Point (BP) domain wall (DW), have gained attention as potential information carriers for nanoelectronic applications due to their high velocity of nearly 2 km/s in the magnonic regime [1, 2]. However, despite ongoing experimental attempts to measure DW velocities, numerical studies that combine both current and Oersted field in nanowires have been scarce[3].

To address this gap, we investigate the BP dynamics under both current and Oersted field in a Ni nanowire using two scenarios: a pre-nucleated BP DW and a transformation of a Vortex-Antivortex DW [4]. Our findings show that the pre-nucleated DW, with the same chirality as the Oersted field, always propagates against the current direction. In contrast, the BP that originates from a DW transformation or a chirality switching can either stop its propagation or move parallel to the current. We also provide the velocities of the BP as a function of the current. Different pinning regimes is contrasted with experimental evidence [5]

In addition, our study reveals that field-driven Bloch point domain walls can reach velocities as high as 14 km/s [6], exceeding the magnonic limit. This is due to the conical shape of the domain wall, which elongates and breaks during the dynamics, resulting in domain wall acceleration through the jet propulsion effect.

Our results lead us to conclude that BPs with vanishing momentum propagate in the opposite direction to the current, and their velocities may be suppressed by the Oersted field. Importantly, we highlight the crucial role of both momentum and inertial mass in the BP dynamics, which has not been fully explored previously and has significant implications for spintronic applications.

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A Theory of Unusual Anisotropic Magnetoresistance in Bilayer Heterostructure

Xiangrong Wang[1, 2,*]
[1] *The Hong Kong University of Science and Technology (Hong Kong)*
[2] *HKUST Shenzhen Research Institute (China)*
* phxwan@ust.hk

Abstract ID #NMM-0824

The observation of magnetoresistance (MR) varying with the rotation of magnetization in the plane perpendicular to the electric current is an important discovery in spintronics in recent years. The famous conventional anisotropic MR (AMR) says that the resistance of a polycrystalline magnetic material must depend on magnetization component along the current direction only, thus cannot account for this newly observed unusual AMR (UAMR). This UAMR leads to the notion of the spin-Hall MR (SMR) in the famous SMR theory. However, the SMR theory may only explain UAMR observed in heavy-metal/magnetic-insulator bilayers, not other types of bilayers. Here, we present a two-vector theory that can explain not only all existing experiments on the unusual angular dependence of longitudinal and transverse resistivity when the magnetization rotates in three mutually perpendicular planes, but also how three amplitudes of MR angular oscillation are related to each other. The theory is general, and its correctness depends only on the assumption that magnetization and interfacial field are the only vectors affecting electron transport. Experiments that can test this theory against the SMR theory are also proposed.

ACKNOWLEDGMENTS

This work is supported by the National Key Research and Development Program(No. 2020YFA0309600), the NSFC Grant (No. 11974296), and HK RGC Grants (No. 16301619, 16300522, and 16302321).

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Magnetic Properties of Two-Dimensional 1T-NiI_2

Andrii Chumak*
University of Vienna, Faculty of Physics, Boltzmanngasse 5, A-1090 Vienna (Austria))
* andrii.chumak@univie.ac.at

Abstract ID #NMM-0825

Yttrium-iron-garnet (YIG) is the ideal choice of material to build and develop classical and novel quantum technologies [1]. Performing propagating spin-wave spectroscopy on thin films at millikelvin temperatures is the next step toward the realization of large-scale integrated magnonic circuits for quantum applications. In the talk, I will demonstrate spin-wave propagation in a 100 nm-thick YIG film at temperatures down to 45 mK [2]. The clear transmission characteristics over the distance of 10 μm are measured from which the extracted spin-wave group velocity and the YIG saturation magnetization agree well with the theoretical values. It was also found that the magnetic moment induced in gadolinium-gallium-garnet (GGG) substrate at low temperature disturbs the magnon transport for the applied magnetic fields beyond 75 mT. To address this phenomenon, the magnetization of the GGG substrate was measured via vibrating-sample magnetometry, and the magnetic properties of the YIG film were characterized by ferromagnetic resonance (FMR) measurements. It is found that the magnetization of GGG results in the formation of a stray field oriented in the opposite direction to the external field. Moreover, the magnetization of GGG increases the magnetic damping of YIG by more than eight times compared to measurements at room temperature.

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Magnetic Skyrmions Probed by Spin-polarized STM: Topology Imprinted on the Charge Current and Spin Transfer Torque

Krisztián Palotás*
Wigner Research Center for Physics, Budapest (Hungary)
* palotas.krisztian@wigner.hu

Abstract ID #NMM-0828

The controlled creation and annihilation of individual magnetic skyrmions have been demonstrated by using spin-polarized scanning tunneling microscopy (SP-STM) [1], where the spin-polarized current exerts a torque on the spin moments of the sample. However, the detailed microscopic mechanism of this process is presently unknown. Our work contributes to this understanding by a theoretical investigation of the tunneling electron charge and spin transport probing magnetic skyrmions. The spin-polarized charge current (I) and tunneling spin transport vector quantities, the longitudinal spin current and the spin transfer torque (STT), are consistently calculated within a simple electron transport theory [2]. The electron tunneling model is extended to SP-STM in high spatial resolution, and applied to magnetic skyrmions [3]. Besides the vector spin transport characteristics, the relationships among conventional charge current SP-STM images [4], the magnitudes of the spin transport quantities [3], and the topology of various skyrmionic objects are analyzed [5]. It is also shown that at specific SP-STM tip positions the STT efficiency (STT/I) can reach very large values ~h/e [5].

ACKNOWLEDGMENTS

Financial support from NKFI OTKA 124100, the János Bolyai Research Grant of the Hungarian Academy of Sciences (BO/292/21/11) and the New National Excellence Program of the Ministry for Culture and Innovation from NKFI Fund (ÚNKP-22-5-BME-282) is gratefully acknowledged.

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How Magnetism Can Improve Rapid Diagnostic Tests: Pneumococcal Pneumonia Detection

María Salvador[1, 2,*], José Luis Marqués-Fernández[1], Alexander Bunge[3], Juan Carlos Martínez-García[1], Rodica Turcu[3], Davide Peddis[4], María del Mar García-Suárez[5], María Dolores Cima Cabal[5], Diana Leitao[6], Montserrat Rivas[1]

[1] *Department of Physics & IUTA, University of Oviedo (Spain)*
[2] *Institute of Material Science of Madrid - CSIC (Spain)*
[3] *National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca (Romania)*
[4] *Department of Chemistry and Industrial Chemistry, Università degli Studi di Genova (Italy)*
[5] *Escuela Superior de Ingeniería y Tecnología, Universidad Internacional de La Rioja (Spain)*
[6] *Applied Physics and Science Education, Eindhoven University of Technology (Netherlands)*
* salvadormaria@uniovi.es

Abstract ID #NMM-0833

The SARS-CoV-2 virus has generated an unprecedented need for rapid diagnostic tests to enable the efficient detection and mitigation of COVID-19 pandemic. In its first stages, the diagnostic was based on PCR or other techniques which were scarce, expensive and with the additional problem of the need of hiring trained personnel. The availability of the gold standard tests used at that time (i.e., PCR) hindered the response in well-funded health care systems. This situation was even more dire in low- and middle-income countries. Lateral flow assays (LFAs) appeared as the most promising rapid tests thanks to their low cost and ease of use. Traditional ones use gold or latex nanoparticles to detect the presence of the molecule of choice. In such a case, LFAs are limited to qualitative detection and lack the necessary sensitivity for low-concentration analysis (giving rise to frequent fake negative results), especially in complex biological matrices. The use of magnetic nanoparticles as detection labels coupled with magnetic sensors would improve both limitations [1].

Developing magnetic LFAs offers advantages (i.e., magnetic concentration of the analyte) and challenges (i.e., optimization for biomarker detection). Then, the quantification of the nanoparticles can be performed by different approaches thanks to the magnetic properties of the labels, which should be addressed without adding excessive complexity to the method. We have developed in our laboratory LFAs for real-world applications. Two recent examples will be presented in this talk: Detecting antibodies generated by SARS-CoV-2 and quantifying pneumolysin, the protein that indicates pneumococcal pneumonia in urine [2] thanks to a radio-frequency inductive sensor based on a planar coil to both excite and detect the particles was used for that purpose. Using magnetic nanoclusters, we proved their ability to concentrate diluted samples thanks to their magnetic character. Thanks to this simple technique, we considerably improved the detection limit for the inductive sensor to 0.2 ng/mL.

ACKNOWLEDGMENTS

This work was partially founded by the Ministry of Science and Innovation of the Spanish Government through grant PLEC2022-009490, the University Technological Institute of Asturias (IUTA), under grant SV-22-GIJON-18, and the Government of the Principality of Asturias underprojects FICYT/IDI/2021/000100 and FICYT/IDI/2021/000273. M.S. was supported by a "SeveroOchoa" fellowship (Consejería de Educación y Cultura del Gobierno del Principado de Asturias, grantBP19-141) and by the Margarita Salas fellowship financed by the European Union-NextGenerationEUand the Plan for Recovery, Transformation and Resilience.

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Semi-Analitycal Model of Topological Magnonic Crystal

Juraj Feilhauer[1,*], Mateusz Zelent[2], Zhiwang Zhang[3], Johan Christensen[4], Michal Mruczkiewicz[1]
[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*
[2] *Faculty of Physics, Adam Mickiewicz University in Poznan, Umultowska 85, Poznan, PL-61-614 (Poland)*
[3] *Department of Physics, MOE Key Laboratory of Modern Acoustics, Collaborative Innovation Center of Advanced Microstructures, Nanjing University (China)*
[4] *IMDEA Materials Institute, Calle Eric Kandel, 2, 28906, Getafe, Madrid (Spain)*
* juraj.feilhauer@savba.sk

Abstract ID #NMM-0836

As one of its most unique features, the bulk of the 2D topological insulator is insulating while its edges host conducting symmetry-protected states robust against imperfections. These edge states are unidirectional (i.e. immune against back-scattering), which makes them promising candidates for the low-dissipation information carriers in future information-processing devices. Topological edge states were demonstrated theoretically and experimentally in many wave-hosting platforms, e.g. electronic systems [1], optical [2] or acoustic crystals [3]. Despite the growing research on topological magnetics, topological edge states in magnonic systems (i.e. hosting spin waves) have not been observed experimentally so far. In 2013, Shindou et al. [4] proposed a theoretical model of a topological magnonic crystal, where the unit cell consists of four spins circulating in-plane coupled solely by magnetostatic dipole interaction. Increasing the out-of-plane magnetic field, the system undergoes several topological phase transitions accompanied by the presence of the unidirectional edge states.

Recently, we have proposed a numerical model of a ferromagnetic artificial crystal hosting topological spin waves (magnons) with simple geometry that should be experimentally realizable [5]. Unit cell of our magnonic crystal is a ferromagnetic square cut along its diagonals into four identical right-angle isosceles triangles. Due to the shape anisotropy, these triangles are naturally magnetized along their bases and their net magnetic moments circulate around the center of the unit cell with the same chirality from cell to cell. Small widths of the lines separating the triangles ensure strong dipolar coupling between them. The lowest-frequency spin wave eigenmode of a single triangular element is well separated from the higher-frequency excitations. In the unit cell, the four lowest-frequency modes of triangles give rise to four azimuthal modes, where the two of them described by a clockwise and counterclockwise phase rotation are degenerated. In the magnonic crystal, these azimuthal modes are dipolarly coupled resulting in four magnonic bands. Increasing the out-of-plane magnetic field, the degeneracy of azimuthal modes is lifted and their order of frequencies can be reshuffled. This is responsible for the band gap closing and subsequent band inversion driving the topological phase transition and emergence of unidirectional edge states.

In this paper, we present an effective semi-analytical model of our topological magnonic crystal inspired by Shindou et al. [4], where the net magnetic moments of triangles are approximated as macrospins and the shape anisotropy of triangular elements is taken into account. This effective model nicely quantitatively reproduces the numerically calculated bandstructure and serves as proof that the macrospin approximation is valid in the case of our magnonic crystal.

ACKNOWLEDGMENTS

The research has received funding from the Slovak Grant Agency APVV (grant number APVV-19-0311(RSWFA)), and VEGA agency, grant number VEGA-2/0177/21. This study was performed during the implementation of the project Building-up Centre for advanced materials application of the Slovak Academy of Sciences, ITMS project code 313021T081 supported by Research & Innovation Operational Programme funded by the ERDF (50%).

The research has received funding from National Science Centre of Poland, Grant No. UMO-2018/30/Q/ST3/00416. The simulations were partially performed at the Poznan Supercomputing and Networking Center (Grant No. 398).

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Using Magnetic Nanowires for Localized Heating

Roman Kolisnyk, Allison Harpel, Yicong Chen, Bethanie Stadler*,
University of Minnesota Twin Cities (United States)
* stadler@umn.edu

Abstract ID #NMM-0840

Magnetic nanoparticles of many kinds have been used for localized heating in electronic [1] and bio-applications [2], where an alternating magnetic field (AMF) induces hysteretic losses in the nanoparticles. Key examples are hyperthermia therapy for cancer [3], rewarming of cryopreserved bio-specimens [4], magnetic detection [5] and melting solder. The critical parameters vary with application, but uniformity and fast warming rates are always desirable. Pioneering studies have superparamagnetic iron oxide nanoparticles (SPIONs) because they are commercially available and FDA approved for experimental studies. However, SPIONs tend to agglomerate due to spherical shapes and easy coherent rotation of their magnetizations, so uniformity remains a challenge. In addition, iron oxide has a relatively low magnetization (0.63T), and super-paramagnetism by definition means and "S" shaped hysteresis loop with limited area except at high frequencies (10-100 kHz). Here, localized heating is explored using magnetic nanowires (MNWs), which range in diameter (10-10000nm) and length (10-200nm) and aspect ratio (0.1-10000). MNWs have up to 4x the magnetization of SPIONS (2.45 for FeCo), and their coercivities are dictated by their magnetic reversal mechanism and diameter. Importantly, most MNWs have rectangular hysteresis loops that enable maximum energy transfer from AMFs because the specific loss power (SLP in W/g) is equal to the area of the hysteresis loop multiplied by frequency. This work focuses on predicting and experimentally verifying trends in SLP using micromagnetic simulations and electrochemical deposition plus characterization of Fe, Ni, Co, FeCo and FeNi MNWs. Surprising trends were found experimentally to show that two distinct magnetic reversal mechanisms exist, and understanding these enables optimization of heat transfer from any user specified AMF amplitude/frequency pair. Two applications are studied in depth: nanowarming of cryopreservation agents and nano-breadboards.

ACKNOWLEDGMENTS

The authors thank AFSOR (FA9550-21-1-0273) and NSF via ATP-Bio (EEC-1941543). Parts of this work were conducted in the Minnesota Nanofabrication Center and Characterization Funding who recieve support from the National Nanotechnology Coordinated Infrastructure (NNCI) under Award Number ECCS-2025124, and in the Institute of Rock Magnetism funded by the University of Minnesota and by NSF (NSF-EAR 1642268; NSF-EAR 2153786).

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Unraveling Interactions Between Magnetic Nanochains for Reconfigurable Soft Actuators

Yulan Chen[1,*], Karthik Srinivasan[1], Marcus Choates[2], Ludovico Cestarollo[1], Amal El-Ghazaly[1]
[1] *Cornell University (United States)*
[2] *The Pennsylvania State University (United States)*
* yc2555@cornell.edu

Abstract ID #NMM-0847

Reconfigurable soft actuators are highly desirable for many applications, including soft robotics, but require more in-depth studies to improve the extent and efficiency of their actuation. Magnetic soft actuators are attractive candidates for this purpose due to the strength and speed of their responsiveness to external magnetic fields. However, relatively little attention has been devoted to the influence of the shape and concentration of the magnetic filler (typically in the form of nanoparticles or other nanostructures) on the properties of the assembled actuator, from its magnetic to its mechanical characteristics. In this study, we synthesized iron cobalt nanostructures including nanoparticles and self-assembled nanochains using a magnetic field-free assembly method. After synthesis a fixation magnetic field was used to align the nanostructures. Though nanochains largely remained in their single-particle-wide form but organized into longer chains separated by regular distances, the synthesized nanoparticles formed multi-particle-wide elongated strands with a width of a few micrometers. In both cases, alignment of the nanostructures led to an augmentation of their collective magnetic properties compared to when they were randomly oriented, with chains demonstrating a more pronounced enhancement (2x) in magnetic remanence. To further investigate the magnetic behaviors of the nanochains, their properties were systematically studied as a function of concentration. It was discovered that there exists a threshold concentration where the interactions between nanochains transition from ferromagnetic coupling to antiferromagnetic coupling. This resulted in a trend of initially increasing and subsequently decreasing remanence and coercivity as the concentration increased. The maximum remanent concentration for a collective magnetic nanochain system was achieved at a filler concentration of 6 vol%, which yielded an Mr/Ms ratio approaching 0.5.

Furthermore, we successfully fabricated a reconfigurable magnetic composite film by incorporating the optimal concentration of magnetic nanochains into an elastomer matrix. An actuator was made with two separate magnetic panels, into which we encoded either the same magnetization directions or opposite magnetizations to achieve various actuation modes. Subsequent reprogramming could be achieved through the application of a magnetic field to one or both panels. This actuator exhibited either S-shaped twisting or U-shaped bending, respectively, in response to the magnetic field (less than 400 Oe) and could be repeatedly reprogrammed. This research emphasizes the potential of magnetic nanochains as effective magnetic fillers and determines the optimal concentration of this magnetic filler for the development of reconfigurable, highly elastic actuators.

Synthesis and Characterization of Magnetic Graphene Based Cation Exchanger for Adsorption of Methylene Blue

Poonam Kumari[1,*], Disha disha[2], Raj Rani[1], Manoj Nayak Kumar[2]
[1] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India (India)*
[2] *CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C Chandigarh (India)*
* p.bangarwa77@gmail.com

Abstract ID #NMM-0849

In recent times, synthetic dyes production has grown exponentially to reach the high demands of industries brought about the natural fall of the textile industry from natural dyes due to profitability. These synthetic dyes are not only used as dyes for the textile, paper, pharmacy, food, leather and cosmetic industries, but also used as a disinfectant in aquaculture and preservative for animal feed. However, it has harmful effects like difficulty breathing, burning, nausea, vomiting and diarrhea. Therefore, there is a need to remove synthetic dyes from wastewater to avoid water related disease and reuse this water for many purposes [1].

This study reports the facile preparation of cation exchange sulfonated magnetic graphene oxide nanoadsorber from oxidized graphene by modifying the Hummers method and its ability to remove synthetic dye methylene blue (MB) from aqueous solutions. Magnetic graphene oxide (MGO) was synthesized by co-precipitated method in presence of Fe^{2+} and Fe^{3+} (1:2) in presence of Graphene oxide (GO) [2]. Further, SMGO was synthesized by EDC/NHS chemistry in presence of 2-amino sulfonic acid. The structure and surface morphology of the SMGO was characterized with XRD, FTIR, Raman, XPS, FESEM, and HRTEM while the magnetic behavior analyzed with VSM and thermal stability using TGA. Various physiochemical parameters such as, dye concentration, contact time, pH of the solution at room temperature were investigated using the batch-adsorption technique [3]. The adsorption of the sulfonic acid functionalized magnetic graphene oxide (SMGO) cation exchanger has been systematically studied, including saturated adsorption capacities, adsorption isotherm and kinetics. SMGO demonstrated a high adsorption efficiency of 225.22 mg g-1 (R2=0.993) for MB dye, due to its good dispersibility as well as multiple adsorption sites. Multiple regeneration experiments indicated that SMGO remained over 80% effective after seven cycles and therefore be used several times. The developed nanoadsorbent SMGO as a low-cost cation exchanger, its easy regeneration, magnetic separation can be used in many various field with well-defined structure.

ACKNOWLEDGMENTS

The authors thank the CSIR-Central Scientific Instruments Organization of Chandigarh for providing facilities for research and funding support from the University Grants Commission of New Delhi, India. Particullary thanks to UGC for providing JRF scholarship.

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Topological Chirality in the Absence of Antisymmetric Exchange

Svitlana Kondovych[1,*], Igor Lukyanchuk[2]
[1] *Institute for Theoretical Solid State Physics, IFW Dresden (Germany)*
[2] *Laboratory of Condensed Matter Physics, University of Picardie, Amiens (France)*
* s.kondovych@ifw-dresden.de

Abstract ID #NMM-0852

The texturing of the vector order parameter in confined ferroics usually arises because of the competing interplay between the dipole-dipole interaction, elastic strains, anisotropic energy, and confinement effects. Nonuniform textures possessing the definite handedness (chirality), – Bloch domain walls, merons, skyrmions, and Hopfions, – attract particular interest due to their fundamental importance and numerous potential applications. Here we consider magnetic [1,2] and ferroelectric [3,4] materials, in which chirality establishes spontaneously in order to reduce the stray fields, even in the absence of chirality-generating local antisymmetric exchange of the Dzyaloshinskii-Moriya type.

The effect is especially pronounced in confined ferroelectrics due to the large electrostatic energy induced by the depolarization field of bound charges. To avoid their formation, a topological constraint of zero field divergence applies to the polarization field. The relevant approach to study fundamental topological structures emerging in a divergenceless vector field was developed by Arnold [5] for topological hydrodynamics. When applied to nanostructured ferroelectrics, the theory predicts the emergence of two types of elementary topological excitations: 2D (achiral) vortex states [6] and 3D (chiral) knotted structures – Hopfions [3].

We focus on ferroelectric nanoparticles hosting chiral topological states and develop the theoretical approach describing their formation. We illustrate the different examples of the confined polar vector fields, revealing the degree of their polarization swirling and handedness.

ACKNOWLEDGMENTS

S.K. acknowledges the support from the Alexander von Humboldt Foundation.

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Spin Wave`s Dynamics in the Two-Sublattice Magnets

Olha Boliasova[1, 2*], Vladimir Krivoruchko[1]
[1] *O.O. Galkin Donetsk Institute for Physics and Engineering , NAS of Ukraine (Ukraine)*
[2] *State Research Institution «Kyiv Academic University» (Ukraine)*
* ol.boliasova@gmail.com

Abstract ID #NMM-0868

In recent years there are highly debates around a new type of future electronic devices. One of the possible candidates for carrying information is spin waves [1]. They have low Joule heating during their propagation which can ensure low energy consumption in computing devices. The next important aspect is the promising high speed of writing/reading information. So now the main challenge is to learn how to manipulate and propagate spin waves.

It was known that spin waves could be manipulated by electric and magnetic fields [2]. For example, they shift the frequency spectrum in horizontal and vertical directions accordingly. However, the electric field could be a more appropriate tool for manipulation. It could create spin-waves with right-handed and left-handed polarization [3] at the same time, it is not necessary to have the inverse breaking symmetry in the two-sublattice magnets.

In addition to the spin-waves spectrum, it is important to consider dissipation processes. One of the well-known phenomenological approaches is based on the Landau-Lifshitz-Gilbert equation. When considering two-sublattice magnetics, the system becomes more complicated, and instead of one damping parameter, four can be considered [4], which significantly affects the dissipation and even the energy spectrum.

Here we provide results that show the importance of including damping parameters. We found that a few Gilbert damping parameters could increase/decrease the frequency`s quantity at the same wave vector. Moreover, it could significantly influence dissipation. At the same time, the behavior of the graphs depends on the relationship between the damping parameters.

Our results demonstrate that damping parameters can play a significant role in the magnetization dynamics. These parameters could influence the practical implementation of a spin wave field-effect transistor [3] or spin wave interferometric devices [5].

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Magnon Dynamics in Anti- and Altermagnets: Long-range Spin Transport, Surface Waves, and Magnon Birefringence

Olena Gomonay*
Institute of Physics, Johannes Gutenberg University Mainz (Germany)
* ogomonay@uni-mainz.de

Abstract ID #NMM-0871

Magnons in antiferro(alter)magnetic materials exhibit the ability to carry two opposite spin polarizations and can effectively transfer spin across long distances. This characteristic makes them highly promising for applications in information encoding and low-energy spintronic devices. In this presentation, I will explore the distinct features associated with the spin transport by magnons in collinear antiferro- and altermagnets. The peculiarities of magnon spin transport in these materials encompass several noteworthy aspects. First, distinct mechanisms govern the long-range spin transport in easy-axis and easy-plane antiferromagnets [1]. In the easy-axis phase, the spin of magnons remains protected by symmetry, enabling their transmission over long distances without any distortions. However, in the easy-plane phase, the anisotropy field influences the rotation of spin [2], resulting in local oscillations of the transport signal that depend on the strength of the magnetic field. Second, in antiferromagnets with Dzyaloshinskii-Moria interactions, the existence of surface waves contributes to the spin transport phenomena [3]. These surface waves arise due to the oscillation of the non-zero magnetization and the accompanying dipole magnetic field. As a result, the propagation of magnons with specific wave vectors becomes confined to the surface. Remarkably, these surface magnons exhibit spin polarization, and their spin polarization is intimately linked to the direction of propagation. Finally, in altermagnets, the spin splitting of electronic bands gives rise to magnons with opposite spins that propagate at different phase and group velocities [4], which results in a magnon birefringence effect when these magnons cross the domain boundary. Additionally, as these spin-split magnons interact with the domain walls, partial reflection takes place, involving momentum transfer. This intriguing phenomenon presents an opportunity for manipulating domain walls and enabling spin switching through the controlled utilization of spin-polarized magnon fluxes. To conclude, our findings highlight the diverse properties exhibited by magnons in antiferromagnetic materials, presenting exciting possibilities for introducing novel functionalities into spintronic devices.

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Design of Magnetic Tunnel Junctions for Microwave Detectors and Physical Unclonable Functions

Mario Carpentieri[1,*], Giovanni Finocchio[2]
[1] *Politecnico di Bari (Italy)*
[2] *University of Messina (Italy)*
* mario.carpentieri@poliba.it

Abstract ID #NMM-0879

Spintronic diodes (SDs) can be considered one of the most promising directions of spintronic technology [1]. Their working principle is based on the rectification of an ac signal with a frequency from MHz to THz. MHz and GHz solutions are realized with magnetic tunnel junctions (MTJs) and, thanks to major breakthroughs in the fabrication of perpendicular MTJs, they can achieve high detection sensitivity (200 kV/W) at room temperature, without bias fields and for low input power (μW or lower) [2].

The presentations will cover different applications of SDs by theoretically and experimentally showing (i) recent advancements in microwave detectors. In addition, a spintronic amplifier with a record gain of 2 for input power on the order of nW (< - 40 dBm) based on two-terminal MTJs will be presented. It is produced with CMOS-compatible material stacks that have already been used for spin-transfer torque memories [3].

Another potential application of MTJs is toward security, by realizing a novel class of Physical Unclonable Functions (PUF). The realization proposed here is based on a three terminal MTJ device where the random bit is written by the spin-hall effect (SHE), while the bit reading is achieved via the magnetoresistive effect. We show the condition to achieve a PUF state with 50% of up and 50% of down state randomly distributed in an MTJ matrix. The proposed low cost and energy efficient device is scalable to be integrated in advanced CMOS technological nodes, reconfigurable, radiation hardness, robust against voltage variations and temperature fluctuations [4].

ACKNOWLEDGMENTS

This work was supported under the project number 101070287 — SWAN-on-chip — HORIZON-CL4-2021-DIGITAL-EMERGING-01, the project PRIN 2020LWPKH7 funded by the Italian Ministry of University and Research., and by the PETASPIN association (www.petaspin.com).

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Characterization of Fe_3O_4-Polyethyleneimine Nanocomposites for Magnetic Harvesting of Freshwater Microalgae

Kristína Gerulová[1], Alexandra Kucmanová[1], Zuzana Sanny[1], Zuzana Garaiová[2], Eugen Seiler[3], Mária Čaplovičová[4], Lubomír Čaplovič[4], Marián Palcut[1,*]

[1] *Faculty of Material Science and Technology in Trnava, Slovak University of Technology in Bratislava, Trnava (Slovakia)*

[2] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*

[3] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[4] *Slovak University of Technology (Slovakia)*

* marian.palcut@stuba.sk

Abstract ID #NMM-0880

Microalgae are single-cell photosynthetic microorganisms with high lipid contents. They are considered as potential resources for biodiesel production and nutrition. The microalgal biodiesel production involves several steps including cell cultivation, harvesting, extraction of lipids, and fatty acid methyl ester generation. The harvesting of microalgae is a challenging process complicated by low biomass concentration in aqueous media. Furthermore, microalgal cells carry a negative surface charge which complicates their harvesting by negatively charged flocculants including Fe_3O_4. In the present work, positively charged Fe_3O_4-polyethyleneimine nanocomposites were prepared and studied for magnetic harvesting of freshwater microalgae. Fe_3O_4 nanoparticles were synthesized by co-precipitation of ferrous (Fe^{2+}) and ferric (Fe^{3+}) salts in aqueous ammonia. Subsequently, the Fe_3O_4 nanoparticles were coated with polyethyleneimine (PEI). The synthesis was carried out at room temperature to decrease the production costs. The prepared nanocomposites were characterized by X-ray diffraction, magnetometry, high-resolution transmission electron microscopy, and zeta potential measurements [1, 2]. Subsequently, the nanomaterials were used for magnetic harvesting of freshwater microalgae. The harvesting efficiencies of PEI-coated Fe_3O_4 were considerably higher compared to bare Fe3O4. Efficiencies up to 99% were achieved in acidic solutions. The results show that magnetic harvesting of freshwater microalgae is feasible and can be enhanced by PEI coating. The coating brings a positive electrical charge to Fe_3O_4 nanoparticles. Furthermore, the magnetic flocculants can be synthesized at room temperature, thereby reducing the costs of the process.

ACKNOWLEDGMENTS

This work received funding from the Slovak Research and Development Agency (project No. APVV-20-0124), Grant Agency VEGA of the Ministry of Education, Science, Research and Sport of the Slovak Republic (projects No. 1/0756/20, 1/0345/22 and 1/0531/22), Grant Agency KEGA of the Ministry of Education, Science, Research and Sport of the Slovak Republic (project No. 020STU-4/2021) and the European Regional Development Fund (ITMS project codes 313021X329 and 313011W085).

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Gigahertz Gyrotropic Excitations in Vortex-State Magnetic Nanodots

Artem Bondarenko[1], Sergey Bunyaev[1], Kostyantyn Gusliyenko[2], Adekunle Adeyeye[3], Gleb Kakazei[4, *]
[1] *Departamento de Física e Astronomia, Institute of Physics for Advanced Materials, Nanotechnology and Photonics (IFIMUP), Universidade do Porto (Portugal)*
[2] *University of the Basque Country, UPV/EHU, San Sebastian and Ikerbasque, Bilbao (Spain)*
[3]*Durham University (United Kingdom)*
[4]*Institute of Physics for Advanced Materials, Nanotechnology and Photonics (Portugal)*
* gleb.kakazei@fc.up.pt

Abstract ID #NMM-0883

Movement towards the 3rd dimension allows obtaining spintronic nanodevices with much richer functionality, compared to traditional realizations in planar 2D magnetic structures. In this work we extend a common two dimensional magnetic vortex structures, known for producing an efficient dynamical response to external stimuli without bias magnetic field, into the 3rd dimension. This extension leads to a drastic vortex frequency increase, up to 5 GHz, contrasted with typical sub-GHz range reported for planar vortex oscillators. A systematic study reveals a complex pattern of vortex excitation modes, which provides explanations for the fall of the thickness-homogenous oscillation mode frequency, vortex mode intensities inversion, and nontrivial spatial distribution of the vortex dynamical magnetization reported in earlier works [1-3]. The observed phenomena allow for optimization of both oscillation frequency and frequency reproducibility (by minimizing the effect of uncontrolled size uncertainties) of such magnetic devices.

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Development of a Magnetic Sensor Using Co:MgO Antidots

Yuan Ding[1], David C. Lloyd[1], Masaki Mizuguchi[2], Masaru Ikeda[2], Atsufumi Hirohata[1,*]
[1] *University of York, York (United Kingdom)*
[2] *Nagoya University, Nagoya (Japan)*
* atsufumi.hirohata@york.ac.uk

Abstract ID #NMM-0888

Magnetic sensors have been widely used to detect a position, an angle and a magnetic field. They mainly use three physical phenomena for sensing: Hall, anisotropic and giant magnetoresistance effects [1]. Hall sensors are most-commonly used but their operation is limited to the temperature range typically between - 40 and 120 ºC with a magnetic field between 102 and 106 Oe. Recently, we have demonstrated a linear response in magnetisation under a small magnetic field up to ± 500 Oe using an antidot array consisting of ferromagnetic Fe nanoparticles dispersed in insulating MgO matrix [2]. In this study, we have adopted a similar antidot with replacing Fe with Co and have characterised the magnetisation dynamics.

We co-deposited Co and MgO at the ratio of 2:1 by electron-beam evaporation on MgO(001) and (011) substrates by ultrahigh vacuum molecular beam epitaxy. The total film thickness was selected to be 30 nm with the epitaxial relationship of Co(001)[010]//MgO(001)[010] as previously reported in Ref. [3]. The antidots were post-annealed at 400 ºC for up to 3 hours in 1 hour steps under a vacuum. All the samples show stronger magnetic anisotropy with the MgO[010] and [100] directions to be the easy and hard axis, respectively. Along the hard axis, the magnetisation curves show almost linear response within ± 750 Oe. Their magnetisation dynamics were also measured by ferromagnetic resonance, showing clear signals at 6~8 GHz.

ACKNOWLEDGMENTS

This study was partially supported by the Royal Society International Exchanges (IEC\R3\203006), EPSRC (EP/V007211/1) and JST CREST (JPMJCR17J5).

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Physical Mechanisms Affecting Performance of Perpendicular STT MRAM Cells

Goran Mihajlović
San Jose Research Center, Western Digital Corporation, San Jose, CA 95119 (United States)
* goran.mihajlovic@wdc.com

Abstract ID #NMM-0890

Spin transfer torque magnetoresistive random access memory (STT MRAM) is an alternative to SRAM [1] and Flash [2, 3] in various embedded applications, as it can provide non-volatility concurrently with low power, high speed operation, and high endurance. In order to become a viable option for replacing DRAM as a stand-alone memory at relevant areal densities, further optimization of MRAM performance is needed, as continued technology scaling and advanced computing systems impose challenging specifications on MRAM in terms of its retention (thermal stability), read-out latencies, and write margins [4]. This talk will present our recent experimental, theoretical, and modeling results on understanding physical mechanisms that affect performance of perpendicular STT-MRAM cells under electrical, magnetic and thermal excitations. In particular, we will report experimental and modeling results that extend of our recent work on electrical self-heating in STT-MRAM [5] to smaller device size, describe our work on optimization of FL materials for improving STT efficiency and thermal stability [6], present analytical model for calculating energy barrier for domain-wall-mediated magnetization reversal of the perpendicular FL [7], and show our experimental results which suggest that, contrary to common understanding, fitting the magnetic-field switching probabilities P(H) to a macrospin-reversal model provides approximately correct values of perpendicular magnetic anisotropy field Hk on device level. Finally, we will show that by increasing the thickness of the MgO cap layer to make its resistance-area product RA close to that of the main MgO barrier, the write margin can be increased substantially for the given write speed and endurance, without affecting thermal stability of the cell in a significant way.

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Analysis of the Possibilities of Using Spin-Valve Structures Based on Fe_xCo_{1-x} and Fe_xNi_{1-x} and Cu as Functional Elements of Spintronics

Alla Saltykova[1,*], Dmytro Saltykov[2], Yurii Shkurdoda[3]
[1] *Sumy State Pedagogical University named after A.S. Makarenko, Romens'ka St. 87, 40002 Sumy (Ukraine)*
[2] *Sumy State Pedagogical University named after A.S. Makarenko, Romens'ka St. 87, 40002 Sumy (Ukraine)*
[3] *Sumy State University, 2, Rimsky-Korsakov St., 40007 Sumy (Ukraine)*
* 0809saltykova@gmail.com

Abstract ID #NMM-0892

Today spintronics needs new materials to create functional elements and devices that will ensure its further development. Among a number of structures that can be effectively used in spintronics, spin-valve type structures based on Fe_xCo_{100-x} and Fe_xNi_{100-x} film alloys and Cu were selected for analysis. Three-layer films based on $FexCo_{100-x}$ (Fe_xNi_{100-x}) with different concentrations of components and a Cu interlayer were obtained by layer-by-layer films condensation of individual layers in a vacuum: Cu by the method of thermal evaporation, alloy films - using electron-beam evaporation. The analysis of literary sources [1-3] and the obtained research results [4, 5] make it possible to find the optimal combination of functional parameters: the value of giant magnetoresistance (GMR), magnetoresistive sensitivity, magnetic hysteresis, the required value of the remagnetization field and high temperature stability. Changing the characteristics is possible by changing the condensation conditions, the thickness of the layers, the elemental composition of their components and heat treatment.

The studied structures have low saturation fields and, as a result, high sensitivity to changes in the magnetic field, which is important when using such structures in devices for recording and reading information. For $Fe_xNi_{1-x}/Cu/Fe_xNi_{1-x}$ systems, at $x > 0.3$, the saturation fields are up to 5 mT, which provides a sensitivity of S_B = (50 – 80) %/T. For $Fe_xCo_{1-x}/Cu/Fe_xCo_{1-x}$ systems, at $x \leqslant 0.5$, the saturation fields are up to 20 mT, and the sensitivity S_B = (50 – 70) %/T.

The advantage of film structures based on an alloy of iron with cobalt or nickel is a rather large time and temperature stability of properties. However, when manufacturing magnetoresistive elements based on structures with a ferrum-cobalt alloy, thermal stabilization annealing in a vacuum at a temperature of 550 K immediately after condensation of the films should be recommended.

Consequently, spin-dependent electron scattering at relatively small magnetic fields is realized in the above-mentioned nanostructures, and they also have high sensitivity to the magnetic field and temporary thermal stability. Such structures can be used in the production of various devices, such as sensors for the magnetic field for cars, the angle of rotation, the speed of rotation and the amplitude of vibrations of objects, etc.

ACKNOWLEDGMENTS

This work was funded by the Project No. 9918 Magnetism in Ukraine Initiative.

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Spin Wave Based Computing: Promises and Hurdles on the Road

Sorin Cotofana
Delft University of Technology (Netherlands)
* S.D.Cotofana@TUDelft.nl

Abstract ID #NMM-0899

In this presentation we provide an overview of recent efforts to develop computing systems based on spin waves instead of charges and voltages. Note that Spin-wave computing can be considered a subfield of spintronics, which uses magnetic excitations for computation and memory applications. We start with an introduction to magnetic interactions, spin-wave physics, and basic spin-wave computing mechanisms. Subsequently, we review individual spin-wave devices while focusing on spin-wave majority gates as they are the most prominently pursued spin-wave device concept. Afterwards, we discuss the current status and the challenges to combine spin-wave gates to obtain circuits and ultimately computing systems, by considering essential aspects, e.g., gate interconnection, logic level restoration, input-output consistency, and fan-out achievement. Then, we argue that spin-wave circuits need to be embedded into conventional complementary metal-oxide-semiconductor (CMOS) circuits to obtain complete functional hybrid computing systems, review the state of the art of benchmarking such hybrid spin-wave-CMOS systems, and discuss challenges towards their practical realization. The benchmark indicates that hybrid spin-wave-CMOS systems promise ultralow-power operation and may ultimately outperform conventional CMOS circuits in terms of the power-delay-area product.

ACKNOWLEDGMENTS

This work has been funded by the European Union's Horizon 2020 research and innovation program within the FET-OPEN Project CHIRON under Grant Agreement No. 801055.

Electron Tunneling and Spin-Dependent Phenomena: Developing Concepts for Random Access Memory

Marek Przybylski
Faculty of Physics and Applied Computer Science, AGH University of Krakow, 30-059 Krakow, Poland (Poland)
* marprzyb@agh.edu.pl

Abstract ID #NMM-0900

The data stored as the magnetization orientation of a ferromagnetic electrode, which is possible in two opposite directions corresponding to logic 0 or 1, results in a different tunneling current detected by the other ferromagnetic electrode of a fixed magnetization. This offers an easy tool for reading the stored data (a concept of magnetic random access memory called MRAM). The realization of this concept (20 years old) is based on tunneling through the MgO barrier; however, the first successful spin-dependent tunneling was realized more than 50 years ago. With ongoing development, it has become possible to replace the magnetic field (originally used for the writing of the magnetization orientation) with a spin-polarized current flowing through the junction (STT-MRAM), and then with the current flowing only through one of the electrodes (SOT-MRAM). However, recent concepts suggest the magnetoelectric or electric writing of the magnetization or the ferroelectric state, respectively, and the inverse-spin Hall effect for reading the stored data. This would make tunnel junctions and spin-dependent electron tunneling unnecessary for future spin-based RAMs. Such RAM devices would be able to switch faster, with lower energy consumption, and being non-volatile at the same time compared to the existing RAM.

The Influence of Temperature on the Processes of Spin-Dependent Electron Scattering in Metal Film Alloys

Larysa Odnodvorets, Yurii Shabelnyk*, Iryna Cheshko
Sumy State University (Ukraine)
* y.shabelnyk@aph.sumdu.edu.ua

Abstract ID #NMM-0902

The giant magnetoresistance (GMR) effect is primarily related to the influence of spins on the electrical conductivity of ferromagnetic metals. The spin-dependent conductivity mechanism is explained by the band structure of a ferromagnetic metal. The splitting of energy levels related to the "up" ("majority spin") and "down" ("minority spin"). This leads to the fact that at the Fermi level, the electrons are in different states that correspond to opposite spin orientations. Such a model of spin-dependent conductivity was proposed by N.F. Mott to explain some features of the electrical resistance behavior of ferromagnetic metals near the Curie temperature. The phenomenon of spin states mixing occurs due to the processes of spin reversals and, mainly, as a result of scattering on magnons, which, increasing with increasing temperature, partially equalizes the currents of the "spin-down" and "spin-up" channels above the room temperature for most ferromagnets.

The ratio for the resistivity of the metal has the form [1]: $1/\rho_0 = 1/\rho_\uparrow + 1/\rho_\downarrow$, where $\rho_\uparrow$ is the resistance of the spin channels with the orientation of the spins "up" and $\rho_\downarrow$ is the resistance of the spin channels with the orientation spins "down". To calculate the resistance of the spin channels, the following values were determined: $\Delta\rho/\rho_0 = \gamma\cdot(\alpha - 1)$ and $\gamma = 3/4\cdot(A/H)^2$, where H is the intensity of the external magnetic field. Coefficient $\gamma \cong 5.5\cdot10^{-4}$ for Fe-based alloys. $\alpha = \rho_\downarrow/\rho_\uparrow$ - is the polarization parameter. Experimental data for the resistivity of spin channels of film alloys based on ferromagnetic metals from work [2] were used for calculations.

Calculated contributions of different spin orientations to the resistivity of film alloys based on Fe and Pd or Pt. We established that for the specific resistance for the "spin-down" state to the specific resistance for the "spin-up" state, $\alpha = 8 - 11$ in the presence of Pt atoms in the Fe film and becomes $\alpha = 20 - 23$ in the presence of Pd atoms.

The two-current model of the conductivity of ferromagnetic films is based on the proposition that electron currents with spin-up and spin-down directions interact by collision with momentum exchange. The phenomenon of mixing of spin states occurs due to the processes of spin reversals and, mainly, as a result of scattering on magnons, which, increasing with increasing temperature, partially equalizes the currents of the "spin-down" and "spin-up" channels above the room temperature for most ferromagnets. The results of calculations for film alloys based on Fe and Pd or Pt indicate a strong scattering of electrons in only one spin channel, leaving the other free, so there is no strong increase in resistance in the magnetic field.

ACKNOWLEDGMENTS

The work was carried out within the framework of the Grant under the "Magnetism for Ukraine 2022" program from the IEEE Magnetics Society and STCU (No. 9918).

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Multicomponent Functional Materials: Kinetic and Magnetoresistive Properties

Serhiy Protsenko, Larysa Odnodvorets*, Yurii Shabelnyk, Olena Lobodiuk, Natalia Shumakova, Ivan Protsenko

Sumy State University (Ukraine)

* l.odnodvorets@aph.sumdu.edu.ua

Abstract ID #NMM-0903

Today, several main types of nano-sized film materials can be distinguished (see, for example, [1, 2]): multilayer film systems and multilayers consisting alternately of magnetic and non-magnetic layers; granular film materials; combined multilayer systems of nanosized magnetic layers in the form of granular nanocomposites of magnetic nanoparticles embedded in a non-magnetic matrix; ordered solid solutions; film alloys with different degrees of entropy.

Multicomponent film alloys are a modern promising class of functional materials in which their kinetic and magnetoresistive properties can be varied within wide limits by changing the condensation conditions, concentration of components, and phase composition. Due to their high temperature stability, multicomponent materials have prospects for use in the formation of elements of integrated microcircuits by the method of multilayer metallization with a predetermined structure of layers and the value of operating parameters, as well as sensitive elements of sensor electronics. This determines the novelty and relevance of the the work.

The goal of the work: forecasting and research of kinetic (resistivity, mean free path of electrons - MFPE) and magnetoresistive (magnetoresistance and giant magnetoresistance - GMR) properties of multicomponent film alloys, including high-entropy, from the point of view of their practical application as elements of sensor electronics.

It is shown that in high-entropy film alloys (HEA) the formation of a stable solid substitution solution (mainly with fcc-, bcc- or (fcc+ccc) lattices) takes place, which is both highly strong and thermodynamically stable, which is explained by the high entropy of mixing atoms.

Studies of the kinetic and magnetoresistive properties of HEA indicate relatively large values of resistivity (10-7 Ohm.m), which can be explained by the defects of the films (vacancies and boundaries between nanocrystallites). It was experimentally established that in HEA films based on Co, Ni, Cu, Fe and Al, the magnetoresistance amplitude at T=300 K is relatively small (0.15-0.40 %).

On the basis of the calculations, the concentration dependences of the resistivity and MFPE for multi-component metal materials with the number of components from 4 to 6 in the form of film or bulk alloys were obtained. Calculations under the assumption of additivity of physical quantities (resistivity, thermal coefficient of resistance and MFPE) for bulk multicomponent materials correspond to experimental data for films HEA (correspondence of results ±5-10 %).

ACKNOWLEDGMENTS

This work was created under the support by ministry of education and science of Ukraine project No 0122U000785 (2022 – 2024 years).

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TRACK 8

“SUPERCONDUCTIVITY IN NANOSCALE & MESOSCOPIC SYSTEMS”

Vortices and Nonequilibrium Phenomena in Nanoengineered Superconductors

Oleksandr Dobrovolskiy*
Faculty of Physics, University of Vienna (Austria)
* oleksandr.dobrovolskiy@univie.ac.at

Abstract ID #SNMS-0489

Fast vortex dynamics and related nonequilibrium phenomena are essential subjects of research in modern superconductivity [1]. High velocities of magnetic flux quanta (Abrikosov vortices or fluxons) attract great interest because of the fundamental questions regarding their stability as topological excitations of the superconducting order parameter and the ultimate speed limits for magnetic flux transport via vortices at intense transport currents [2]. Furthermore, fast dynamics of fluxons determines the vortex-assisted mechanism of the initial dissipation of superconducting microstrip single-photon detectors (SMSPDs) [3] and makes accessible novel phenomena, such as the generation of sound and spin waves in superconductor-based heterostructures [4].

In may talk, which will serve as an overview for the Focus Session on Nanoengineered Superconductors, I will introduce two complementary research directions in superconductivity and fluxonics: (i) Dynamics of the topological modes in superconductor 2D and 3D nanoarchitectures and (ii) Nonequilibrium states occuring in superconductor-based structures at large dc currents, high ac frequencies, and in consequence of photon absorption. The ultimate speed limit for fluxons plays an essential role for the performance of these applications, as it roots in the fundamental microscopic mechanisms of the relaxation of quasiparticles (unpaired electrons). However, the deduction of the maximal vortex velocity v* from the current-voltage (I-V) curves at zero magnetic field (SMSPD operation condition) is hindered by the unknown number of vortices, as a small number of fast-moving vortices, n_v, can induce the same voltage as a large number of slow-moving ones.

To provide a solution to this problem, I will dwell more on our recent results regarding the quantitative determination of n_v and v* [5]. The idea is based on the observation of kinks in the I-V curves of wide and short superconducting constrictions when the number of fluxons crossing the constriction is increased by one. We realize such conditions in wide MoSi thin strips with slits milled by a focused ion beam and reveal quantum effects in a macroscopic system. By observing kinks in the I-V curves with increase of the transport current, we evidence a crossover from a single- to multifluxon dynamics and deduce v*~12 km/s. Our experimental observations are augmented with numerical modeling results, which reveal a transition from a vortex chain over a vortex jet to a vortex river with increase of n_v and v. Our findings are essential for the development of one-dimensional and two-dimensional few-fluxon devices and provide a demanded approach for the deduction of maximal vortex velocities at the SMSPD operation conditions.

ACKNOWLEDGMENTS

This research is funded in whole, or in part, by the Austrian Science Fund (FWF), Grant Nos. I 6079-N (FluMag) and I 4865-N (FluxPin), and is based upon work from COST Actions CA19108 (HiSCALE) and CA21144 (SuperQuMap), supported by COST (European Cooperation in Science and Technology).

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Ising Superconductivity in Bulk Materials

Tomas Samuely[1,*], Darshana Wickramaratne[2], Martin Gmitra[3,4], Thomas Jaouen[5], Ondrej Šofranko[6], Dominik Volavka[6], Marek Kuzmiak[4], Jozef Haniš[6], Pavol Szabó[4], Shunsuke Sasaki[7], Laurent Cario[7], Igor Mazin[8], Peter Samuely[4]

[1] *Centre of Low Temperature Physics, Faculty of Science, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia (Slovakia)*
[2] *Center for Computational Materials Science, U.S. Naval Research Laboratory, Washington (United States)*
[3] *Institute of Physics, Pavol Jozef Šafárik University in Košice (Slovakia)*
[4] *Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)*
[5] *Univ Rennes, CNRS, (IPR Institut de Physique de Rennes) (France)*
[6] *Centre of Low Temperature Physics, Faculty of Science, Pavol Jozef Šafárik University in Košice (Slovakia)*
[7] *Institut des Matériaux Jean Rouxel, Université de Nantes and CNRS-UMR 6502 (France)*
[8] *Department of Physics and Astronomy and Quantum Science and Engineering Center, George Mason University (United States)*

* tomas.samuely@upjs.sk

Abstract ID #SNMS -0522

Low-dimensional materials can exhibit remarkable properties different from their bulk counterparts. $NbSe_2$ monolayer is an Ising superconductor with the in-plane upper critical field violating the Pauli limit, while no such behavior occurs in bulk $NbSe_2$ [1]. However, in contrast to bulk, low-dimensional materials are often unstable and impractical for applications. Utilizing various experimental techniques, we found that $(LaSe)_{1.14}(NbSe_2)$ and $(LaSe)_{1.14}(NbSe_2)_2$ bulk layered misfit superconductors exhibit a two-dimensional band structure equivalent to a highly doped $NbSe_2$ monolayer [2]. Moreover, their in-plane upper critical fields exceed the Pauli limit by a factor of up to 10 [3]. From first-principles calculations backed by experimental results we obtained their detailed band structure parameters, such as the values of the reduced interlayer coupling and strong spin-orbit splitting. This quantitative analysis enabled us to explain the microscopic origin of the Ising spin-orbit coupling in bulk superconductors.

ACKNOWLEDGMENTS

This work was supported by the projects APVV-20-0425, VEGA 2/0058/20, EMP-H2020 Project No. 824109, COST action CA21144 (SUPERQUMAP), EU ERDF (European regional development fund) Grant No. VA SR ITMS2014+ 313011W856.

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Disorder- and Magnetic Field-Tuned Fermionic Superconductor-Insulator Transition in MoN Thin Films. Transport and STM studies

Pavol Szabó*
Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)
* pszabo@saske.sk

Abstract ID #SNMS -0531

Superconductor-insulator transition (SIT) driven by disorder and transverse magnetic field has been investigated in ultrathin MoN films by means of transport measurements and scanning tunneling microscopy and spectroscopy. Upon decreasing thickness, the homogeneously disordered films show increasing sheet resistance Rs, shift of the superconducting transition Tc to lower temperatures with the 3 nm MoN being the last superconducting film and thinner films already insulating. Fermionic scenario of SIT is evidenced by applicability of the Finkelstein's model, by the fact that Tc and the superconducting gap D are coupled with a constant ratio, and by the spatial homogeneity of the superconducting and electronic characteristics. The logarithmic anomaly found in the tunneling spectra of the non-superconducting films is further enhanced in increased magnetic field due to the Zeeman spin effects driving the system deeper into the insulating state and pointing also to fermionic SIT. The results presented in this contribution are the first complete studies of the disorder and magnetic field induced fermionic superconductor-insulator transition using transport and local STM measurements on samples from both sides of the SIT.

Anisotropic Vortex Squeezing and Supercurrent Diode Effect in Non-Centrosymmetric Rashba Superconductors

Denis Kochan*
Institute of Physics, Slovak Academy of Sciences (Slovakia)
* denis.kochan@savba.sk

Abstract ID #SNMS -0567

Most of 2D superconductors are of type II, i.e., they are penetrated by quantized vortices when exposed to out-of-plane magnetic fields. In a presence of a supercurrent, a Lorentz-like force acts on the vortices, leading to drift and dissipation. The current-induced vortex motion is impeded by pinning at defects. Usually, the pinning strength decreases upon any type of pair-breaking interaction perturbs a system.

In the talk I will discuss surprising experimental evidences showing an unexpected enhancement of pinning in synthetic Rashba 2D superconductors when applying an in-plane magnetic field. When rotating the in-plane component of the field with respect to the driving current, the vortex inductance turns out to be highly anisotropic. We explain this phenomenon as a direct manifestation of Lifshitz invariant that is allowed in the Ginzburg-Landau free energy when space-inversion and time-reversal symmetries are broken. As demonstrated in our experiment [1], elliptic squeezing of vortices---an inherent property of the non-centrosymmetric superconducting condensate---provides an access to fundamentally new property of Rashba superconductors, and offers an entirely novel approach to vortex manipulation.

Another interesting feature of the non-centrosymmetric superconductors in the applied magnetic field is the supercurrent diode effect---the critical current in one direction exceeds its counterpart in the opposite one---what stems from the Cooper pairs with finite centre of mass momentum. In the pioneering experiment [2] we demonstrated the emergence of the supercurrent diode effect in the Josephson junctions based on synthetic Rashba superconductors made of Al-InAs quantum wells. In the talk, I will discuss novel experimental method---measurements of the Josephson inductance---and the semiquantitative microscopic model capturing all the essential features as observed in experiment.

ACKNOWLEDGMENTS

This research was partly supported and funded by

1) IMPULZ project IM-2021-26---SUPERSPIN funded by the Slovak Academy of Sciences,

2) VEGA Grant No.~2/0156/22---QuaSiModo funded by The Ministry of Education, Science, Research and Sport of the Slovak Republic,

3) Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) within Project-ID 314695032---SFB 1277.

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Nanofabrication of Curvilinear and 3D Superconducting Architectures

Rosa Córdoba*
University of Valencia (Spain)
* rosa.cordoba@uv.es

Abstract ID #SNMS -0575

Superconducting materials are dissipationless carriers of electric current and provide macroscopic and robust quantum coherence. These properties render them highly valuable as parts for electrical generators, magnetic sensors, and powerful magnets. To achieve the required performance employed in those applications, bulk superconductors often need nanoengineering. Moreover, when these materials are reduced to the nanoscale becoming nano-superconductors, exciting new physical phenomena emerge.

Ground-breaking proposals have taken advantage of the third dimension (3D) for the development of advanced electronic components, opening fascinating novel routes in the fields of material science, physics and nanotechnology. Thus, 3D nano-superconductors could be implemented in future highly-efficient electronic elements. However, their fabrication and characterization remain a challenge.

In this contribution, we introduce a direct-write additive manufacturing method based on focused ion beam technologies to fabricate at-will advanced nano-superconductors.

We have prepared 3D superconducting hollow nanocylinders with controllable inner and outer diameters (down to 32 nm), and nanohelices with at-will geometries, by decomposing a precursor with a He+ FIB [1,2]. These nanostructures become superconducting at 7 K and show large critical magnetic field and critical current density. Remarkably, these nanohelices display superconductivity up to 15 T depending on the direction of the field with respect to the nanohelix axis. This suggest that their helical 3D geometry and their orientation in a magnetic field play a significant role in the superconducting phase transition. Moreover, fingerprints of vortex and phase-slip patterns are also experimentally identified and supported by numerical simulations based on the time-dependent Ginzburg-Landau equation [3]. Additionally, we present an experimental work on the modulation of electric field-induced superconductivity in 45 nm-wide nanowires fabricated using Ga+ FIB [4], theoretically explained using a model based on the GL theory [1].

ACKNOWLEDGMENTS

COST Action, FIT4NANO STSM; SEJIGENT 2021/012, Generalitat Valenciana; Ramón y Cajal Contract 2021, MICIIN

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Size Effects and Excess Noise in Superconducting Nanowire Single-Photon Detectors

Mariia Sidorova[1,*], Sebastian Raupach[2], Alexei Semenov[3]
[1] *Nanyang Technological University (Singapore)*
[2] *Physikalisch-Technische Bundesanstalt (PTB) (Germany)*
[3] *German Aerospace Centre (DLR) (Germany)*
* mariia.sidorova@ntu.edu.sg

Abstract ID #SNMS -0577

Superconducting Nanowire Single-Photon Detectors (SNSPDs) offer unique performance such as extended spectral sensitivity (from visible to near-infrared range), low dark count rate (1 dark count per hour), and high timing resolution (a few picoseconds) making them highly desirable for applications in quantum computing, quantum communication, and quantum/classical light detection. However, new sophisticated applications such as deep-space communication or direct detection of dark matter particles require even more stringent performance criteria from the SNSPD technology. Among others, they require extremely low, if any, dark count levels and broad spectral sensitivity up to the middle infrared range. We identify new strategies for improving the overall performance of these devices from a material science perspective by investigating size effects and excess noise in superconducting nanowires.

The photon detection mechanism in a current-carrying superconducting nanowire is relatively simple. An absorbed photon with energy largely exceeding the superconducting gap locally breaks superconductivity that eventually drives the nanowire into the resistive state which is experimentally registered as a photon count. The dynamics of this process is governed by phonons and electron systems and thermal coupling to the substrate. The miniaturization of device sizes in superconducting nanoelectronics, particularly in SNSPDs, which are conventionally made of 5 nm-thick and 100 nm-wide superconducting nanowires, leads to modification of their thermal properties at low temperatures. The reciprocal film thickness limits the phonon wave vectors perpendicular to the film plane, significantly altering the phonon spectrum and the heat capacitance of phonons. Our extensive studies of superconducting NbTiN films [1, 2] with polycrystalline granular morphology revealed the impact of mean grain size on the phonon heat capacitance. Such size effect can be used to tune the cut-off in the spectral sensitivity of SNSPDs via engineering the phonon properties.

In SNSPDs, besides stochastic dark counts caused by thermal fluctuations [3], there are conditional dark counts, or afterpulsing [4], as a kind of excess noise that presents a significant challenge in improving device performance. We observed that the probability of an afterpulse in an SNSPD made of amorphous MoSi depends on the mean number of photons per light pulse, including values much less than one. Our proposed phenomenological model explains our findings by introducing slowly relaxing afterpulsing centers, which we believe may be two-level systems in amorphous materials. While two-level systems are well-known sources of decoherence and losses in superconducting qubits and resonators, their impact on SNSPD performance is yet to be explored. Therefore, understanding the microscopic details and material science aspects may play a dominant role in further improving the performance of superconducting devices.

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Superconductor 3D Nanoarchitectures: Properties due to Complex Geometry and Nontrivial Topology

Vladimir M. Fomin*
Leibniz Institute for Solid State and Materials Research (IFW) Dresden (Germany)
Moldova State University, Chişinău (Republic of Moldova)
* v.fomin@ifw-dresden.de

Abstract ID #SNMS -0592

Extending nanostructures into the third dimension has become a major research avenue in condensed-matter physics, because of geometry- and topology-induced phenomena. Modern advances of high-tech fabrication techniques have allowed for generating geometrically and topologically nontrivial manifolds at the nanoscale, which determine novel, sometimes counterintuitive, electronic, magnetic, optical and transport properties of such objects and unprecedented potentialities for design, functionalization and integration of nanodevices due to their complex geometry and non-trivial topology [1]. In open superconductor Nb nanotubes with a submicron-scale inhomogeneity of the normal-to-the-surface component of the applied magnetic field, a topological transition between the vortex and phase-slip regimes determines the magnetic-field-voltage and current-voltage characteristics, which imply a possibility to efficiently tailor the superconducting properties of nanostructured materials by inducing a nontrivial topology of superconducting screening currents [2]. Most of peaks in the induced-voltage-magnetic-field characteristics appear in the presence of abrupt switch-on of the transport current or the magnetic field. Such an abrupt switch-on triggers the transition from the vortex to phase-slip regime. The dependence of the superconducting regimes on the switch-on speed and the stability of such regimes hints that there is a barrier between them. As the result, a novel hysteresis effect is unveiled in the current-voltage characteristic of open nanotubes [3]. The hysteresis loop is wider in current, but narrower in voltage for a stronger magnetic field. Normal conductivity has a crucial impact on the hysteresis effect in superconductor open nanotubes. Namely, a higher normal conductivity leads to the disappearance of the hysteresis effect. As a rule, the upper and lower branches of the hysteresis loop are provided by the phase-slip and vortex regimes, correspondingly. Just before the transition of the system from the upper branch to the lower one, the way of nucleation and annihilation of vortices in the region with suppressed superconductivity experiences readjustment [4]. Dynamic topological transitions in open superconductor nanotubes occur under a combined dc+ac transport current [5]. The key effect is a transition between two regimes of superconducting dynamics. The first regime is characterized by a pronounced first harmonic in the FFT spectrum of the induced voltage at the frequency of the ac current. It occurs when the dominant area of the open tube is superconducting at relatively low magnetic fields and/or weak dc currents - or normal at relatively high magnetic fields and/or strong dc currents. The second regime manifests a rich FFT spectrum of the induced voltage with pronounced multiple harmonics of the ac frequency because of an interplay between the internal dynamics of superconducting vortices or phase slips and the dynamics driven by the ac.

ACKNOWLEDGMENTS

I acknowledge fruitful collaborations with O. V. Dobrovolskiy, R. O. Rezaev and I. Bogush. This work was supported by the DFG (Germany) under Project No. FO 956/6-1 and by the European Cooperation in Science and Technology via the COST Action CA21144 "SUPERCONDUCTING NANODEVICES AND QUANTUM MATERIALS FOR COHERENT MANIPULATION" (SUPERQUMAP).

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Interplay of Superconducting Gap and Spin-Orbit Coupling in Rhombohedral Graphite Proximitized by $NbSe_2$

Zoltán Tajkov[1,*], Marko Milivojević[2], Martin Gmitra[3,4]
[1] *Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences, Košice SK-04001, Slovakia (Slovakia)*
[2] *Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia (Slovakia)*
[3] *Institute of Physics, Pavol Jozef Šafárik University in Košice (Slovakia)*
[4] *Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)*
* tajkov@saske.sk

Abstract ID #SNMS -0616

In recent years, there has been growing interest in the study of the interplay of different superconducting gap opening functions and induced spin-orbit coupling in novel materials, which has led to the discovery of a number of exotic quantum phenomena. Rhombohedral graphite is a promising candidate for such studies, owing to its unique crystal structure and electronic properties. We investigate the superconducting properties of rhombohedral graphite that is proximitized by a thin film of $NbSe_2$. We use first-principles calculations based on density functional theory to study the electronic properties of this system, and employ a combination of analytical and numerical techniques to analyze the interplay between different superconducting gap opening functions and spin-orbit coupling. In the talk we discuss how the interplay can lead to the emergence of topological superconductivity in the system, which could have important implications for the development of future quantum technologies.

ACKNOWLEDGMENTS

This work was supported by the Slovak Academy of Sciences project IMPULZ IM-2021-42, project FLAG ERA JTC 2021 2DSOTECH, Slovak Research and Development Agency provided under Contract No. APVV-SK-CZ-RD-21-0114, and VEGA 1/0105/20. MM ackownledges SASPRO 2 COFUND Marie Sklodowska-Curie grant agreement No. 945478.

$Bi_2Sr_2CaCu_2O_8$ Thin Film Fabrication for Nanostructuring to Investigate Vortex Dynamics

Sandra Keppert[1,*], Bernd Aichner[2], Wolfgang Lang[2], Johannes Pedarnig David[1]
[1] *Johannes Kepler Universität (Austria)*
[2] *Faculty of Physics, University of Vienna (Austria)*
* sandra.keppert@jku.at

Abstract ID #SNMS -0638

We report on the growth and characterization of the quasi-2D high-Tc superconducting material $Bi_2Sr_2CaCu_2O_8$+d (Bi-2212). Due to its extremely high anisotropy of the electronic and thermal transport properties, it can be considered a quasi-2D material with a layered unit cell structure. We optimized the pulsed laser deposition parameters to grow c-axis oriented and phase pure Bi-2212 films with thicknesses well below 50 nm. Films are characterized via x-ray diffraction, electron microscopy, atomic force microscopy, element analysis and resistivity measurements with and without applied magnetic field. These optimized films will be used for studying vortex dynamics by creating artificial pinning landscaped by ion irradiation in the future.

ACKNOWLEDGMENTS

Financial support by the Austrian Science Fund FWF (project FluxPin,project number I 4865-N) is gratefully acknowledged.

Non-destructive Nanostructuring: Using a Focused Helium Ion Beam to Change the Properties of Cuprate Superconductors

Bernd Aichner[1,*], Max Karrer[2], Katja Wurster[2], Lucas Backmeister[1], Philipp Alexander Korner[1], Barbora Budinská[1], Oleksandr Dobrovolskiy[1], Reinhold Kleiner[2], Edward Goldobin[2], Dieter Koelle[2], Wolfgang Lang[1]

[1] *Faculty of Physics, University of Vienna (Austria)*
[2] *Physikalisches Institut, Center for Quantum Science (CQ) and LISA+, Universität Tübingen (Germany)*
* bernd.aichner@univie.ac.at

Abstract ID #SNMS -0655

Nanostructuring of thin film materials has increasingly drawn attention throughout the last years. One application is the production of pinning structures for magnetic flux quanta in superconductors, such as holes in a thin film or defects in the material. While such structures can be created by lithographic techniques in classical superconductors, their applicability in the cuprate high-critical temperature superconductors is limited since these materials are prone to oxygen loss. This demands a method of locally suppressing superconductivity without damaging the film's surface.

One method suitable for achieving this goal is irradiation with 30 keV helium ions, which suppresses the superconductor's critical temperature Tc in the irradiated region while preserving the material's crystal structure. Here, we present ultra-dense regular structures for pinning magnetic flux quanta in the high-temperature superconductor $YBa_2Cu_3O_{7-\delta}$ (YBCO) created by irradiation in a helium ion microscope. Systematic studies show that the superconductor's electronic transport properties depend on the irradiation fluence and enable us to perform computer simulations of Tc-suppression that are calibrated with experimental data. Having a technique for locally reducing the critical temperature of YBCO to a desired value opens up a vast range of possibilities for manipulating magnetic flux quanta, which has, for example, lead to an ordered Bose glass phase [1,2] in thin films structured with this method.

Altogether, this establishes the method of irradiation in a helium ion microscope as a promising and versatile tool for creating dense and complex structures in high-Tc superconductors, which could be an important step on the way toward low-dissipative superconducting electronics.

ACKNOWLEDGMENTS

This work is funded by a joint project of the Austrian Science Fund (FWF), grant I4865-N, and the German Research Foundation (DFG), grant KO 1303/16-1, and is based upon work from COST Actions CA21144 (SuperQuMap), CA19108 (Hi-SCALE), and CA19140 (FIT4NANO), supported by COST (European Cooperation in Science and Technology).

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Vortex Counting and Velocimetry for Slitted Superconducting Thin Strips

Barbora Budinská[1,*], Volodymyr Bevz[2], Mikhail Mikhailov[3], Sebastian Lamb-Camarena[1], Stanislava Shpilinska[4], Andrii Chumak[5], Michal Urbanek[6], Markus Arndt[6], Wolfgang Lang[1], Oleksandr Dobrovolskiy[1]

[1] *Faculty of Physics, University of Vienna (Austria)*
[2] *V. N. Karazin Kharkiv National University (Ukraine)*
[3] *B. Verkin Institute for Low Temperature Physics and Engineering, NAS of Ukraine (Ukraine)*
[4] *University of Vienna (Austria)*
[5] *University of Vienna, Faculty of Physics, Boltzmanngasse 5, A-1090 Vienna (Austria)*
[6] *CEITEC BUT, Brno University of Technology (Czech Republic)*

* barbora.budinska@univie.ac.at

Abstract ID #SNMS -0670

The research on superconducting microstrip single-photon detectors (SMSPDs) opened a promising route to high system detection efficiency single-photon detectors covering a large active area. An important criterion to be met for the material candidates for SMSPDs is a fast device recovery time correlated to a low intrinsic energy relaxation time τ. Amongst the methods to deduce τ from experiment is performing current-voltage (I-V) measurements and taking note of the voltage just before the flux flow instability (FFI) that causes a voltage jump into the normal state [1]. However, at low and zero magnetic fields this approach fails to deduce physically plausible results. The problem arises given the fact that the number of vortices, deduced from the applied magnetic field only, is in fact larger. Current flowing through the sample nucleates vortices in numbers that are in the same order of magnitude as vortices created due to low applied magnetic fields, and thus cannot be neglected as in the case of higher magnetic fields [2]. Here, we provide a method to count the number of vortices present in the sample just before the FFI at zero magnetic fields. Experiments were performed on a 15 nm-thick MoSi sample with a focused ion beam milled out slit [3]. As predicted by Aslamazov and Larkin, voltage kinks in the I-V curves appear every time the number of vortices crossing from the slit to the opposite edge is increased by one [4]. Thus, the number of voltage kinks corresponds to the number of vortices present. This newly obtainable information allows one to correct the previously unphysical estimates of energy relaxation times τ, and the correlated maximal vortex velocity v*, at low magnetic fields. We believe that this method is of importance not only for a highly demanded approach to assess the suitability of materials for SMSPDs but deepens the knowledge about vortex dynamics and vortex presence for the operation of future few-fluxon devices.

ACKNOWLEDGMENTS

This research is funded in whole, or in part, by the Austrian Science Fund (FWF), Grant Nos. I 6079-N (FluMag) and I 4865-N (FluxPin). This article is based upon work from COST Actions CA19108 (HiSCALE) and CA21144 (SuperQuMap), supported by COST (European Cooperation in Science and Technology).

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The Impact of Solution Treatment on the Properties of High-Temperature Superconductor $YBa_2Cu_3O_{7-x}$

Michal Bennar[1,*], Stefan Chromik[1], Marianna Španková[1], Marcel Talacko[1], Juraj Kronek[2]
[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*
[2] *Polymer Institute of Slovak Academy of Sciences (PI SAS) (Slovakia)*
* michal.bennar@savba.sk

Abstract ID #SNMS -0688

Perovskite oxides are known for a broad variety of unique properties. One of these novel properties is high-temperature superconductivity, which has yet to be theoretically explained. High-temperature superconductor $YBa_2Cu_3O_{7-x}$ (YBCO) is one of the most studied materials. It was discovered early on that most of its electrical properties strongly depend on doping. Doping itself can be changed during time when YBCO is exposed to air, water, and other chemicals [1]. In some applications, there is a need to treat the material with a solution. However, with this arises a problem of interaction between the solvent and the surface layer.

In our study, we investigated the interaction between different solvents and YBCO thin films. YBCO thin films were immersed in the solvents overnight, and the obtained structures were characterized from an electrical and morphological point of view. One surprising result was when YBCO was immersed in dichloromethane. YBCO locally incorporated chlorine into its structure, leading to an increase of critical temperature and critical current density. M. Chen et al. found out that adding chlorine into precursor during the ex-situ growth process yielded the increase of critical temperature, too [2]. It should be noted that the incorporation of chlorine during the growth process [2] and its application in our case represent distinct processes.

ACKNOWLEDGMENTS

This work was supported by the Slovak Research and Development Agency, APVV-19-0303, APVV-16-0315, Slovak Grant Agency for Science, VEGA 2/0140/22.

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Ultrastrong Magnon-Photon Coupling and Entanglement in Superconductor/Ferromagnet Nanostructures

Mikhail Silaev*
Tampere University (Finland)
* mikesilaev@gmail.com

Abstract ID #SNMS-0721

Ultrastrong light-matter coupling opens exciting possibilities to generate squeezed quantum states and entanglement. Here I propose a way to achieve this regime in superconducting hybrid nanostructures with ferromagnetic interlayers [1,2]. Strong confinement of electromagnetic field between superconducting plates is found to result in the existence of magnon-polaritons. These modes provide a numerically accurate explanation of recent experiments and have intriguing quantum properties. The magnon-polariton quantum vacuum consists of the squeezed magnon and photon states with the degree of squeezing controlled in wide limits by the external magnetic field. The ground state population of virtual photons and magnons is shown to be very large, which can be used for generating correlated magnon and photon pairs. Excited states of magnon-polaritons contain bipartite entanglement between magnons and photons. This property can be used for transferring entanglement between different types of quantum systems.

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Time-Dependent Ginzburg-Landau Simulations of Curved 3D Nanoarchitectures

Axel Johan Marie Deenen*, Arnaud Emile S. Nizet, Dirk Grundler
School of Engineering, Institute of Materials, Laboratory of Nanoscale Magnetic Materials and Magnonics, École Polytechnique Fédérale de Lausanne (EPFL) (Switzerland)
* axel.deenen@epfl.ch

Abstract ID #SNMS -0727

Recent advances in nanofabrication have spurred interest in the field of superconductivity in (curvilinear) 3D nanoarchitectures [1]. Additionally, simulations using Time-Dependent Ginzburg-Landau (TDGL) theory have become an essential tool for interpreting experiments on superconductors. However, common implementations of the TDGL in curved 3D geometries either focus on systems that can be mapped to a 2D film, or make use of finite-difference methods which are not well suited for modelling curved geometries. Here, we present finite-element simulations of 3D superconducting geometries with curvature using the TDGL formalism. We implement the formalism in COMSOL Multiphysics and, following Ref. [2], fully take into account the effect of screening currents by computing the magnetic field in both the superconductor and the surrounding vacuum. This approach allows us to capture the dynamic behavior of flux-vortices in type-II superconductors beyond planar geometries.

In our simulations, we place four interconnected type-II superconducting tubes inside a volume of vacuum whose boundaries are sufficiently far such that effects of screening are negligible there. Applying a homogeneous magnetic field we demonstrate the nucleation of vortices at selected locations depending on its magnitude and direction. Additionally, we simulate a Möbius strip consisting of a type-II superconductor and demonstrate the coexistence of the Meissner phase and vortices.

To conclude, by using the finite-element method and a two-domain simulation setup, we model the behavior of superconductors in non-trivial 3D nanoarchitectures. The implementation is an important step towards a better understanding of new phenomena at the mesoscopic scale in the field of 3D superconductivity.

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Non-linear Electrical Transport in Pulsed Magnetic Fields on Superconducting Thin Films

Christopher A. Mizzi[1,*], Fedor F. Balakirev[1], Ivan Nekrashevich[2], Maxime Leroux[3], Masashi Miura[4]

[1] *Materials Physics and Applications-MAGLAB, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 (United States)*

[2] *Superconducting Quantum Materials and Systems Center (SQMS), Fermi National Accelerator Laboratory, Batavia, IL 60510 (United States)*

[3] *LNCMI-EMFL, CNRS UPR3228, Univ. Grenoble Alpes, Univ. Toulouse, Univ. Toulouse 3, INSA-T, Grenoble and Toulouse (France)*

[4] *Graduate School of Science and Technology, Seikei University, Tokyo (Japan)*

* mizzi@lanl.gov

Abstract ID #SNMS -0870

Non-linear electrical transport is indispensable for fundamental research and technological applications of superconductors, especially for studying micro- and nano-scale inclusions, disorder, criticality, and vortex physics. Since large sections of many superconducting phase diagrams occur at very high magnetic fields (H) only attainable in pulsed magnets, non-linear transport capabilities must be developed that are compatible with the strict operating conditions of pulsed magnets. Short pulse durations (~50 ms) and large dH/dt values (~10^4 T/s) are perhaps the most difficult technical challenges for performing pulsed fields experiments. In this talk, I will share recent developments in efficient, non-destructive, non-linear electrical transport measurements in pulsed fields at the National High Magnetic Field Lab's Pulsed Field Facility. We are now able to collect, and immediately analyze, non-linear electrical transport data utilizing the entire field range (55 T) accessible within a single pulse [1, 2]. I will demonstrate our capabilities with critical current and critical field measurements on $YBa_2Cu_3O_{7-x}$ thin films possessing artificial micro- and nano-scale pinning centers.

ACKNOWLEDGMENTS

This work was supported by the Los Alamos National Laboratory LDRD program, project number 20210320ER. The National High Magnetic Field Laboratory, which hosts the high magnetic field magnets, is funded by NSF Cooperative Agreements No. DMR-1157490 and No. 1164477, the State of Florida and Department of Energy.

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TRACK 9

“NANOSENSORS & NANODEVICES”

Development of Biocompatible Piezoelectric Thin Films: Towards a Wearable Sensor Devices

Svitlana Kopyl
University of Aveiro (Portugal)
* svitlanakopyl@ua.pt

Abstract ID #NN-0480

Recently, the focus of research has turned to biomolecular piezoelectrics with sufficiently high piezoelectric properties and intrinsic compatibility with the biological environment. It is based on the complex dipolar properties and dipole-dipole interactions conjugated with hydrogen bonds network in biomolecular systems with different levels of self-assembly and hierarchy. Piezoelectricity in biological objects was found in a number of biological materials of different natures. It is inevitable that such a high coupling will be present in more simple bioorganic materials such as amino acids and peptides. However, only recently emergent piezoelectric properties ($d_{24} \approx 190$ pm/V) have been discovered in crystalline glycine [1]. The voltage piezoelectric coefficient (needed for biomedical applications is 8 V/mN, i.e. several orders of magnitude higher than in the previously used P(VDF-TrFE)]. Recent investigations show that this material can be prepared and stabilized in a thin film form and it is full of ferroelectric domains that can be used as movable conducting interfaces.

Strong piezoelectricity (of the order of that in the classical transducer material $LiNbO_3$) has been discovered in bio-inspired nanotubes made by a self-assembly process of diphenylalanine monomers [2]. These peptide nanotubes (PNTs) originate from the smallest recognition motif of the amyloid-Aβ protein, associated with over 30 neurodegenerative diseases, such as Alzheimer's, Parkinson's, etc. They are made of amino acids, which are self-assembled in unique stable tubes with hydrophilic hollows, having high Young's modulus and profound chemical stability. Recent efforts of our team from the University of Aveiro have focused on understanding the strong piezoelectric properties of peptide nanostructures, prototyping, and optimizing growth conditions [3, 4]. A major problem is an inability to control the self-assembly process to produce dense films with controlled orientation and thickness. To overcome this, we propose a novel method of the formation of crystalline piezoactive FF films via solid phase crystallization directly from the amorphous phase [5]. The process starts with the spin-coating of FF monomers in an organic solution. These layers are then exposed to a controlled humidity that triggers nucleation and growth of highly oriented piezoactive areas (domains). The crystallization process proceeds without changing the morphology and results in dense films with controlled thickness. Large ferroelectric-like domains possess uniform piezoresponse of about 30 pm/V with the in-plane polarization. The growth kinetics is controlled by the temperature and humidity, suggesting that fully in-plane oriented films can be obtained. This is a promising result for the development of multifunctional devices to meet various application requirements, which is an important development trend nowadays.

ACKNOWLEDGMENTS

This work was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020, UIDP/50011/2020 & LA/P/0006/2020, financed by national funds through the FCT/MEC (PIDDAC). This work was developed within the project BioPiezoSensor/2022.03781.PTDC, is financially supported by national funds (OE), through FCT/MCTES.

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Multifunctional Devices Based on 3D Hybrid Networks of ZnO and 3D Carbon Nanomaterials

Armin Reimers[1], Vasile Postica[2], Yogendra Kumar Mishra[3], Adrian Bîrnaz[4], Ali Shaygan Nia[5], Xinliang Feng[6], Rainer Adelung[7], Fabian Schütt[8], Oleg Lupan[9,*]

[1] *Christian-Albrechts Universität zu Kiel Kiel, Germany (Germany)*
[2] *Technical University of Moldova Chisinau, Republic of Moldova (Republic of Moldova)*
[3] *University of Southern Denmark (Denmark)*
[4] *Center for Nanotechnology and Nanosensors Technical University of Moldova Chisinau, Republic of Moldova (Republic of Moldova)*
[5] *Center for Advancing Electronics Dresden (cfaed) Technische Universität Dresden, Dresden, Germany (Germany)*
[6] *Technische Universität Dresden, Dresden, Germany (Germany)*
[7] *Department of Materials Science, Chair for Functional Nanomaterials, Faculty of Engineering, Kiel, Kaiserstraße 2, D-24143 Kiel, Germany (Germany)*
[8] *Faculty of Engineering Christian-Albrechts Universität zu Kiel Kiel, Germany (Germany)*
[9] *Technical University of Moldova (Republic of Moldova)*
* lupanoleg@yahoo.com

Abstract ID #NN-0496

Rapid progress in the field of nanotechnology has led to the development of a large variety of novel nanomaterials with unique sensing properties for application in gas sensing, environmental monitoring and breath analysis [1], photodetectors [2,3] and more [4]. The clever use and combination of these nanomaterials can provide opportunities for the development of new multifunctional high-performance devices [5]. However, the efficient combination of 2D and 3D materials in order to obtain strong synergistic effects and tunable sensing properties is a challenging task.

In this work, the room temperature UV and gas sensing properties of the three-dimensional (3D) networks based on zinc oxide (ZnO) tetrapods coated with carbon-based two-dimensional (2D) nanomaterials were investigated. Therefore, highly porous (~94%) cylindrical pellets of ZnO tetrapods were infiltrated with dispersions of graphene oxide (GO), electrochemically exfoliated graphene (EG) and reduced graphene oxide (rGO), resulting in the formation of nano-porous few-layer membranes on the surfaces of the individual tetrapods, that affect both, their gas and UV sensing properties. It was found, that by coating ZnO with rather insulating materials such as GO, the UV response of ZnO networks can be improved from ~5 to ~17 at an applied bias voltage of 10 V. On the other hand, the addition of conductive carbon-based nanomaterials, such as EG and rGO, results in a decrease in UV response compared to the pristine ZnO networks. The decrease is associated with the formation of percolating pathes through the ZnO network, that shunt the effect of potential barrier modulation between the ZnO tetrapods under UV illumination. However, while decreasing the UV response, EG enabled gas sensing. The EG based 3D networks were capable of detecting NH3 at room temperature, showing a gas response of ~1.15. The gas response could even be slightly increased by removing the underlying ZnO template, creating ultra-lightweight NH3 sensors.

This study illustrates, that creating 3D hybrid networks based on ZnO and carbon based 2D nanomaterials has huge potential for synergistic effects that achieve new unique sensing properties at room temperature.

ACKNOWLEDGMENTS

We acknowledge funding within the project "SuSiBaBy" - SulfurSilicon Batteries by the WTSH and EFRE in SH (LPW-E/3.1.1/1801). We are especially grateful to the Federal Ministry of Education and Research by funding the former "PorSSi" project (03XP0126 A & B). This work was partially supported by the ANCD-NARD Grant No. 20.80009.5007.09 at TUM. Financial support by the project EU-project SENNET "Porous Networks for Gas Sensing", which runs under the Marie Skłodowska-Curie Actions funded by the European Union, under the number 101072845.

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Free Standing Mechano-luminescent Polystyrene/ZnS:Mn Composite Thin Films for Optical Sensing Application

Pallavi Sharma[1,*], Sudipta Sarkar Pal[2], Sachin Tyagi[2]
[1] *Academy of Scientific and Innovative Research (India)*
[2] *Central Scientific Instruments Organisation, Chandigarh, India (India)*
* pallavi.sharma59@yahoo.com

Abstract ID #NN-0511

Mechanoluminescence (ML) phenomenon, is a light generation with the effect of applied mechanical force. The phenomenon is not new but has already been studied by many researchers [1]. Approximately, 50% organic, and 60% of in-organic materials are mechano-luminescent in nature [2]. ZnS:Mn is one of the in-organic phosphor material with the brightest ML signal. Yet, ML sensors are still not available on the market due to a lack of understanding in device fabrication [3][4][5]. Present work focused on the development of Polystyrene (PS)/ZnS:Mn-based composite ML thin films. PS was chosen because it is optically transparent and does not interfere with the phosphor material's optical emission. The film fabrication was done using the drop-casting method and the resulting films are free-standing in nature. The ML films are characterised using Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD) and Photoluminescence (PL) analytical techniques. Further, the composite films are tested for the ML characteristic using a customized pressure pulse generator. The pressure range for testing is set from 40bar to 400bar [6]. The obtained results clearly show that the composite films are ML in nature. The ML is in a linear relationship with the applied pressure as proposed by the theory. These films have a tendency to be utilized for the self-triggered light emission optical sensor matrix material in the areas like Aeronautical, civil structure health monitoring and defence application.

ACKNOWLEDGMENTS

The authors would like to pay the highest gratitude to Director DRDO-Terminal Ballistics Research Laboratory, Chandigarh and Director CSIR-Central Scientific Instrument Organization for the support and encouragement provided to carry out the research work simultaneously in both organizations. Also, the authors would like to thank the scientific team of the Photonics division DRDO-TBRL for support in experimentation. At last, author is also thankful to DRDO for granting a fellowship.

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Facile Reductive Synthesis and Characterization of Heterostructure Core-Shell Silver-Silica Nanocomposite for Humidity Sensing

Fatai Oladipupo Oladoyinbo[1,*], Felix Olaniyi Sanni[1], Fatai Akinwunmi[1], Kamoli Akinwale Amusa[1], Saheed Adekunle Ganiyu[1], Quwam Olamilekan Yusuf[1], Wasiu Babatunde Ayinde[2], Tajudeen Adeniyi Afolabi[1], Enock Olugbenga Dare[1]

[1] *Federal university of Agriculture, Abeokuta, Ogun State (Nigeria)*
[2] *University of Cape Town (South Africa)*

* oladoyinbofo@funaab.edu.ng

Abstract ID #NN-0527

Silver (Ag) and silica (SiO_2) nanoparticles were synthesized using chemical reduction method from silver nitrate and sodium silicate respectively. X-ray Diffraction (XRD), High Resolution Transmission Electron Microscopy (HRTEM), Scanning Electron Microscopy (SEM), Uv-Visible spectroscopy, Energy Dispersive X-ray (EDX) spectroscopy and N_2 adsorption-desorption techniques were utilized to characterize the composition and structure of the samples. Crystallinity pattern of Ag nanoparticles was indexed as (111), (200), (220) and (311), which allowed reflections from face-centred cubic silver. XRD of SiO_2 showed good porosity with broad - spectrum band at Bragg's angle 2θ of 22° while that of Ag-SiO_2 showed distinct peaks at 2θ values of 39°, 43°, 66° and 79°. The XRD result agreed perfectly with the SEM and HRTEM images which showed Ag-SiO2 isotropic and anisotropic under varying concentration of reactants. Elemental composition of Ag-SiO_2 as displayed by EDX confirmed Ag enrichment in the Ag-SiO_2 heterostructure. The Uv-Visible peak at 421 nm confirmed the Surface Plasmon Resonance absorption peak of silver nanoparticles. N_2 adsorption-desorption result showed a broad band of Ag-SiO_2 from 3 to 8 nm which indicated relatively narrow pore size distributions. Humidity sensing measurements performed in a controlled humidity chamber very high sensitivity with sensitivity factor (SF) of 4.63 and high linearity with steady decrease in resistance to humidity from 880 Ω at 10% RH to 190 Ω at 100% RH, indicating that Ag-SiO_2 nanocomposite is a good sensing material with high sensitivity and linearity.

ACKNOWLEDGMENTS

This work was funded by the Tertiary Education Trust Fund (TETFUND) of Nigeria (through Institutional Based Research Grant to FO Research Team). We thank the Federal University of Agriculture, Abeokuta for the Institutional support. We thank the Federal Government of Nigeria for the award of Batch B of TETFUND 2018-2022 Intervention in Research Project IBR Grant for the completion of this work.

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Segregated Polyethylene/Carbon Black Composites for Embedded Heating and Strain Sensing Elements

Yevheniia Buinova[1,*], Anastasiia Kobyliukh[2], Oleksii Maruzhenko[1], Yevgen Mamunya[3], Maksym Iurzhenko[1], Marcin Godzierz[4], Sébastien Pruvost[5], Olha Masiuchok[1], Roman Kolisnyk[1]

[1] *E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine (Ukraine)*
[2] *Center of Polymer and Carbon Materials, Polish Academy of Sciences; Institute of Macromolecular Chemistry, National Academy of Sciences of Ukraine (Poland)*
[3] *Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine (Ukraine)*
[4] *Center of Polymer and Carbon Materials, Polish Academy of Sciences (Poland)*
[5] *Université de Lyon, CNRS, Université Claude Bernard Lyon 1, INSA Lyon, Université Jean Monnet, UMR 5223, Ingénierie des Matériaux Polymères, F-69621 Villeurbanne Cédex, France (France)*
* be.jenn@icloud.com

Abstract ID #NN-0536

The quality control of welded joints is a crucial part of industrial production and can be done by their real-time monitoring. In this study, the potential application of high-density polyethylene-based composites with various carbon black (CB) addition (from 20 to 30 vol.%) for use as an embedded heating element and strain sensor was examined. The pyroresistive heating process was used to determine the impact of generated Joule heat during welding on the structure and piezoresistive properties of composites. It is shown that generation of Joule heat affects the crystallinity of the polymer matrix and partially disrupts the conductive CB path, but that dependents on the CB amount. For lower amounts of CB conductivity decreases after welding, while for the highest CB amount conductivity increases. This phenomenon is related to particle-to-particle distance, which is lower if the volume is higher. Therefore, the best balance between pyroresistive and piezoresistive properties after heating was found as 25 vol.% of carbon black.

ACKNOWLEDGMENTS

The work was performed as a part of Yevheniia Buinova's scholarship for Young Ukrainian Scientist funded by the Polish Academy of Science in cooperation with National Academy of Science of Ukraine.

Authors gives personal thanks to Ukrainian Armed Forces for providing save life.

Influence of the Hydrogen Gas Concentration on the Resistive Switching in the Pt/TiO_2/Pt Memristor

Marek Vidiš[1], Michal Patrnčiak[1,*], Martin Mosko[1], Andrej Plecenik[1], Leonid Satrapinskyy[1], Tomáš Roch[1], Pavol Ďurina[1], Tomáš Plecenik[2]

[1] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*
[2] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava, Mlynska dolina F2, Bratislava 84248 (Slovakia)*

* patrnciak4@uniba.sk

Abstract ID #NN-0549

A recently introduced two-terminal device called gasistor [1] combines a chemiresistive gas sensor and a memristor to achieve a gas sensor with intrinsic memristive memory. Exposure of the metal-oxide chemiresistive gas sensor to oxidizing and reducing gases induces a change of the metal-oxide resistance. At constant current bias, this leads to a change of the voltage applied to the gasistor, i.e. to the gas sensor and memristor. It has been shown in [1] that the induced voltage change may trigger a resistive switch from the high-resistance to low-resistance state, which provides the gasistor with its memory function. Specifically, the gasistor can store in its resistive state the information whether a pre-set hydrogen gas concentration has been reached anytime during its operation.

Such a gas-induced resistive switch has been shown experimentally in a single Pt/TiO_2/Pt cell by reducing the concentration of hydrogen in the air from 10 000 ppm to 0 ppm. However, specific limitations of the device and influence of the hydrogen concentration on the resistive switching parameters of the device haven't been studied yet.

Here we show how various hydrogen concentrations affect the electrical transport characteristics of the gasistor in both high-resistance and low-resistance state and we study their impact on the resistive switching parameters. It has been demonstrated that the resistive switching can be performed in the hydrogen concentration up to 5 000 ppm in synthetic air, depending on the relative resistances of the memristive and gas sensing part of the gasistor. A correlation between the gasistor's sensitivity and the resistance of the device before and after electroforming has been studied.

These results are expected to provide deeper understanding of the gasistor devices and pave the way for development of production-ready gasistors for numerous applications such as gas quality control in industry, long-term surveillance of environmental hazards, or as a thyristor-like gas-controlled switches.

ACKNOWLEDGMENTS

This work was supported by the Slovak Research and Development Agency under the contract No. APVV-21-0053 and by the Scientific Grant Agency of the Slovak Ministry of Education, Sciences, Research and Sport (Grant No. VEGA 1/0062/22). It is also the result of support under the Operational Program Integrated Infrastructure for the projects: Advancing University Capacity and Competence in Research, Development and Innovation (ACCORD) and UpScale of Comenius University Capacities and Competence in Research, Development and Innovation (USCCCORD, ITMS 2014+: 313021BUZ3), co-financed by the European Regional Development Fund.

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Hybrid Metasurfaces Based on Laser-Structured Substrates and Plasmonic Nanoparticles for the Enhancement of Adenosine Nucleotide Raman Spectra

Nataliya Berezovska[1,*], Igor Dmitruk[1], Oleg Yeshchenko[1], Vladislav Kudrya[1], Oleksandr Stanovyi[1], Sergii Golovynskyi[2], Anastasiya Tomchuk[1], Yevhen Hrabovskyi[1], Junle Qu[2]

[1] *Faculty of Physics, Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *College of Physics and Optoelectronic Engineering, Shenzhen University (China)*
* nataliya.berezovska@knu.ua

Abstract ID #NN-0614

The design of promising new structures to facilitate effective detection of nucleic acid bases, which are building blocks of the genetic code, is appropriate for development. The plasmonic cavity metasurfaces based on metal laser-induced periodic surface structures (LIPSSs) and non-spherical metal nanoparticles were shown to provide the highly sensitive detection and imaging of biomolecules at room temperature without their special labelling [1]. Moreover, Raman spectroscopy gives the characteristics of the vibrational modes which are the unique fingerprints of the molecules. The wayfinding to enhance Raman signals to study the structure and interaction of nucleotides, in particular, has been implemented using surface-enhanced Raman scattering (SERS) [2-4]. Here we show the analysis of obtained enhancement of Raman scattering of 5′-deoxyadenosine monophosphate (dAMP) deposited on two types of fabricated cavity metasurfaces, namely: 1) the silver (Ag) LIPSSs and Ag triangular nanoprisms, 2) crystalline silicon (Si) LIPSSs and a pre-deposited thin gold (Au) film modified during laser treatment. Both types of the metasurfaces contain metal or metal-semiconductor substrates which are processed with femtosecond laser radiation in a single step that simplifies the samples formation. The fabricated LIPSSs have the submicron periods. Raman spectra of dAMP on Ag LIPSS/Ag nanoprism metasurface have been measured at excitation wavelengths of 532 and 785 nm at different alignment of Ag ripples. An enhancement of up to 7-fold for the Raman signal for some vibrational modes of dAMP was achieved for 532 nm excitation. In the case of Au NPs/Si LIPSS metasurface we did not achieve sufficiently high enhancement of Raman spectrum of dAMP. This effect additionally emphasizes the crucial role of the near-field coupling of the localized surface plasmon modes of Ag nanoprisms and the propagating surface plasmon polaritons of Ag surfaces and consequent formation of collective plasmonic modes of the entire plasmonic cavity that determine the appearance of hot spots at such metasurfaces. First of all, such hot spots can appear at the edges of non-spherical metal nanoparticles and tips of the LIPSS ripples. Further elaboration of proposed hybrid metasurfaces based on laser-structured substrates and plasmonic nanoparticles could help more detailed understanding of numerous physical and chemical factors such as geometry and optical properties of the metasurfaces based on metal or semiconductor substrate and metal nanoparticles, concentration and orientation of absorbed molecules, chemical environment. This research is perspective, since various SERS-based sensor platforms are being actively developed for the detection of, for example, DNA and RNA bases [5].

ACKNOWLEDGMENTS

The authors appreciate funding from the Ministry of Education and Science of Ukraine (Project No. 0122U001956), the National Research Foundation of Ukraine (Project No. 2020.02/0022) and technical support of Femtosecond Laser Centre for Collective Use of NAS of Ukraine.

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Determination of Carbamazepine Using Luminescent Bifunctional Silica-Based Sensor

Halyna Yankovych*, Inna Melnyk
Institute of Geotechnics SAS (Slovakia)
* yankovych@saske.sk

Abstract ID #NN-0620

The development of a reliable, sensitive and simple analytical technique for the detection and quantitative determination of drugs and their residues is an important issue of analytical and environmental chemistry. The considerable risks of pharmaceutical pollution cause a load on the environmental microbiome and further on the human body [1]. Among a large number of drugs, carbamazepine is a widely used antiepileptic drug that has been detected in water sources in the concentration range 0.035 to 6.3 $\mu g \cdot L^{-1}$ [2], posing a threat to human health and the environment [3] The development of sensitive and reliable methods for the detection of carbamazepine in water is essential for monitoring and controlling its levels. Most of carbamazepine determination methods require special expensive equipment and highly skilled operators that causes additional expenses. To overcome these limitations, luminescence can be used. This analytical method possesses high signal intensity, specificity, selectivity and high sensitivity, and is easy-to-operate.

In the last few decades, the considerable attention is paid to the nanoparticles based luminescent sensors that combine the strong luminescence emission and high quantum yield, longer sensor lifetime and possibility of controllable synthesis and functionalization [4]. Silica based nanomaterials have a great potential due to a flexibility of the synthesis route that allows obtaining particles with the desired size and shape, surface area and controllable surface features. To improve the selectivity and sensitivity of the sensor materials, the modification of nanoparticles' surface with a fluorescent dye is a promising approach owing to the combination of the features of both components, which increases the quantum yield and reduces the luminescence quenching in silica nanoparticles-dye system.

The present research deals with the synthesis of bifunctional silica particles with 3-aminopropyl and phenyl groups modified with Rhodamine 6G (Rh6G) to be applied in luminescent determination of carbamazepine. The materials fabrication was performed by the anchoring of Rh6G to the surface of bifunctional silica by two routes: adsorption of the dye and direct incorporation of dye during the synthesis of silica. Three materials were produced - $SiO_2 \equiv Si(CH_2)_3NH_2/ \equiv SiC_6H_5$, $SiO_2 \equiv Si(CH_2)_3NH_2/ \equiv SiC_6H_5$+$Rh_6G$ (ads.) and SiO2 ≡ Si(CH2)3NH2/ ≡ SiC6H5+Rh6G (synt.). The best sensor response was obtained for the SiO2≡Si(CH2)3NH2/≡SiC6H5+Rh6G (ads.) sample in the concentration range of 0.8-200.0 μM. The estimated limit of detection was 6.0 μM and the limit of quantification was found to be 18.1 μM. The fabricated luminescent sensor is easy to synthesize and operate and possesses a satisfactory result in qualitative and quantitative determination of carbamazepine by simple, fast and reliable analytical procedure.

ACKNOWLEDGMENTS

The research carried out within the APVV-19-0302 project and Štefan Schwarz Postdoc Fellowship No. 2022/OV1/010.

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Combining Gas Sensing and Resistive Switching: Toward Chemiresistive Gas Sensors with Intrinsic Memory

Tomáš Plecenik[1,*], Marek Vidiš[2], Michal Patrnčiak[2], Martin Moško[2], Leonid Satrapinskyy[2], Tomáš Roch[2], Pavol Ďurina[2], Andrej Plecenik[2]

[1] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava, Mlynska dolina F2, Bratislava 84248 (Slovakia)*

[2] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*

* tomas.plecenik@fmph.uniba.sk

Abstract ID #NN-0626

Intelligent gas sensors capable of processing and storing the sensed information are increasingly demanded in environmental monitoring and various areas of industry. However, currently available sensors do not have such capabilities on their own and have to rely on significant amount of additional electronics, which results in increased costs and energy consumption.

Here we show that chemiresistive gas sensors with built-in memory can be obtained by combining gas sensing and resistive switching within a single MIM cell [1]. Such devices, which we call "gasistors", can store in their resistance state the information whether a pre-set threshold concentration of the target gas has been reached anytime during the device operation. On the example of the capacitor-like Pt/TiO_2/Pt gas sensor/memristor we show experimentally that the resistance state of the device can be switched from the high resistance to low resistance state by changing the H_2 gas concentration in the surrounding atmosphere. The threshold concentration at which the switch is triggered can be adjusted by the value of the bias current. Such gas-triggered resistive switching has been manifested in a wide range of temperatures, humidity levels and H_2 gas concentrations. Besides the operation principle of the gasistor devices we further discuss their fundamental limitations and propose ways of their mitigation.

We anticipate that the gasistor devices can play a significant role in long-term monitoring of environmental hazards and various technological processes. Moreover, their incorporation into the memristor-based intelligent gas sensors capable of in-sensor computing can also be expected.

ACKNOWLEDGMENTS

This work was supported by the Slovak Research and Development Agency under the contract No. APVV-21-0053 and by the Scientific Grant Agency of the Slovak Ministry of Education, Sciences, Research and Sport (Grant No. VEGA 1/0062/22). It is also the result of support under the Operational Program Integrated Infrastructure for the projects: Advancing University Capacity and Competence in Research, Development and Innovation (ACCORD) and UpScale of Comenius University Capacities and Competence in Research, Development and Innovation (USCCCORD, ITMS 2014+: 313021BUZ3), co-financed by the European Regional Development Fund.

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Response Characteristics of Hydrogen Gas Sensor Based On Pt-TiO_2-Pt Sandwich Structure With Nanoporous Top Electrode

Michal Patrnčiak[1], Ľubomír Staňo[1,*], Marek Vidíš[1], Leonid Satrapinskyy[1], Tomáš Roch[1], Pavol Ďurina[1], Tomáš Plecenik[2]

[1] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*
[2] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava, Mlynska dolina F2, Bratislava 84248 (Slovakia)*

* lubomir.stano@fmph.uniba.sk

Abstract ID #NN-0627

Chemiresistive gas sensors based on semiconducting materials gained importance in detection of gases and their mixtures in various industrial applications. High sensitivity, short response time and simple peripheral instrumentation are the most remarkable advantages. For reducing gas detection, such as hydrogen, the principle is typically based on reaction of oxygen that is adsorbed to the surface of semiconductor grains. It has been shown that sandwich arrangement of such sensors can enhance their sensitivity due to the strong electric field in the region between the electrodes which can induce a change of the conduction mechanism from thermionic emission to electron drift, if the top electrode is very narrow (< ~200 nm) [1]. However, the very small width of the top electrode can lead to extremely high baseline resistance above the measurement limit of most experimental setups. Such very narrow top electrodes also need to be fabricated by e-beam lithography which complicates the fabrication process and makes it more expensive. On the other hand, wider electrodes lead to decreased response and regeneration time which is caused by long diffusion path of hydrogen molecules within semiconductor grains.

In this work, we aim to solve both above mentioned problems by replacing the very narrow top electrode by a large-scale nanoporous electrode. We demonstrate this approach on a Pt-TiO_2-Pt sandwich structure consisting of a continuous bottom Pt electrode, nanocrystalline TiO_2 layer and a nanoporous top Pt electrode. Both Pt (30 nm) and TiO_2 layers were prepared by DC magnetron sputtering in inert (Ar) and reactive ($Ar+O_2$) atmosphere, respectively, while the nanoporous top Pt layer was obtained by annealing the PtO_x layer deposited by reactive DC sputtering at temperatures of around 660 °C. The dynamic responses of the prepared sensors to hydrogen were measured at various temperatures and humidity levels to demonstrate their functionality in real conditions. The results show that the response $S \geqslant 105$ ($S = R_{air}/R_{H2}$) to 10 000 ppm H_2 and the detection limit below 3 ppm H_2 can be reached by such sensors even at ambient temperature, which could greatly limit the energy consumption of the potential devices. At 150 ° C the response to 10 000 ppm H_2 was as high as 8×10^7. At the same time, the simplified fabrication process is expected to reduce the production costs.

ACKNOWLEDGMENTS

This work was supported by the Slovak Research and Development Agency under the contract No. APVV-21-0053 and by the Scientific Grant Agency of the Slovak Ministry of Education, Sciences, Research and Sport (Grant No. VEGA 1/0062/22). It is also the result of support under the Operational Program Integrated Infrastructure for the projects: Advancing University Capacity and Competence in Research, Development and Innovation (ACCORD) and UpScale of Comenius University Capacities and Competence in Research, Development and Innovation (USCCCORD, ITMS 2014+: 313021BUZ3), co-financed by the European Regional Development Fund.

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Directional Topology Optimization Method in Desing of Anisotropic MEMS Devices

Hossein Rostami Najafabadi[1,*], Thiago Martins[2], Ahmad Barari[1]
[1] *Ontario Tech University (Canada)*
[2] *Escola Politecnica da Universidade de Sao Paulo (Brazil)*
* hossein.rostaminajafabadi@ontariotechu.net

Abstract ID #NN-0639

Topology optimization is a powerful method in the automatic design of structures with optimized performance. Most of the available topology optimization algorithms use the thermal and mechanical properties of a material with an isotopic model. The isotropic model considers the same values for properties of a material in all directions. In the design of MEMS devices, the structural material is mostly silicon with anisotropic properties. This paper applies a directional topology optimization method using simulated annealing to reach the optimum design while the properties of the material are anisotropic. The algorithm has been applied to the design of a microbeam for minimizing compliance with the anisotropic modulus of elasticity for silicon. The results showed a good convergence to the optimum solution while using the maximum capacity of material in the strongest direction.

SARS-CoV-2 Spike Protein Detection Using Silver-Doped Zinc Oxide Tetrapods as SERS Substrate

Edgars Vanags*, Ivita Bite, Annamarija Trausa, Karlis Vilks, Krisjanis Smits
Institute of Solid State Physics, University of Latvia (Latvia)
* edgars.vanags@cfi.lu.lv

Abstract ID #NN-0646

The COVID-19 pandemic has highlighted the need for rapid, accurate, and cost-effective diagnostic methods for biomedical samples, despite the numerous diagnostic techniques available in medicine [1-3]. Surface-enhanced Raman spectroscopy (SERS) has been recognized as a potential technology for testing due to its high sensitivity and selectivity. However, the development of easily accessible point-of-care testing solutions based on SERS technology is currently lacking [4-5].

To address this issue, this study aims to investigate the potential of silver-doped zinc oxide tetrapods as SERS substrates for the specific detection of biomolecules, particularly the spike protein of the virus.

Silver-doped zinc oxide tetrapods were synthesized using the solar physical vapor deposition method and were characterized using SEM-EDX, STEM, XRD, and Raman spectroscopy. The tetrapods were then employed to develop SERS substrates for detecting SARS-CoV-2 spike protein. The eligibility of the silver-doped zinc oxide tetrapods as SERS substrates for the detection of SARS-CoV-2 spike protein was evaluated.

ACKNOWLEDGMENTS

The work has been financed by the European Regional Development Fund Contract No. 1.1.1.1/21/A/053 «The development of a novel-designed optical fiber-based system for ultra-sensitive point-of-care viral protein detection by SERS» and is gratefully acknowledged.

The Institute of Solid-State Physics, University of Latvia as the Center of Excellence has received funding from the European Union's Horizon 2020 Framework Programme H2020-WIDESPREAD-01-2016-2017-TeamingPhase2 under grant agreement No. 739508, project CAMART2.

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FinFETs versus GAAFETs Performances and Perspectives

Arezki Benfdila*
Mouloud Mammeri University, Tizi-Ouzou (Algeria)
* benfdila@ummto.dz

Abstract ID #NN-0697

The present paper deals with a comparative study and investigation on device performances and evaluation trigate FinFETs and gate-all-around FETs. GAAFET are considered as immediate successors of advanced FinFET and nanoMOSFET for next generation of advanced non planar CMOS technology. The present study is carried out on different technology nodes mainly, FinFET and GAAFET and then scaled down respectively. After a physical analysis of both devices, they are modeled and analyzed using SILVACO ATLAS 3D simulation tools for comparison of devices characteristics and technology nodes. It has been found that for the next few years, FinFET 5th generation will be more suitable for CMOS technology; however GAAFET will be the unique devices for the next few decades before graphene and other emerging materials era.

At the nanometric scale, the On-current becomes strongly unbalanced by the phenomena of quantum mechanics. Physical modeling of transistors such as nanowire FETs and FinFETs, simulation techniques based on Monte Carlo finite element set methods and dealing with quantum effects. This is done using the Schrödinger equation at nanometric scale and implementing the gradient density (DG) approach for finite element and finite difference methods and its application in drift-diffusion (D-D) simulations. Numerical models of ballistic and quasi-ballistic transport which exploit the Boltzmann transport equation (BTE).

As a next step, highly and lightly doped GAA NW and FinFET devices were studied for their immunity to variations generated by the fluctuation of doping concentration. A study carried out on the static RAM of the generation of 32/28 nm CMOS technology, shows that discrete doping atoms directly affect their performance.

Design using GAA silicon nanowire transistor (SiNW) process flow can be integrated with proportional density targets as needed, for CMOS technology to evolve downing the10 nm nodes in terms of higher performances.

The results obtained by the simulation process of FinFET and GAAFET devices by the 3D Silvaco technology computer-aided design (TCAD) are found efficient using the Drift-Diffusion (DD) model. The total current density at any point of the FinFET and GAAFET structures is found after resolution of free electron concentrations and holes, using potential and variable parameters such as mobility, electric field and generation-recombination rate…

As a conclusion, the GAAFET NW and FinFET device architectures are studied for different technology nodes. A comparative study based on device performances of two nodes demonstrates that GAA NWs type design is wider and more efficient in performances than FinFETs.

3D Advanced CMOS Technology and Applications

Arezki Benfdila*
Mouloud Mammeri University, Tizi-Ouzou (Algeria)
* benfdila@ummto.dz

Abstract ID #NN-0698

The present talk addresses the development of CMOS technology from classical (planar) to advanced (3D) technologies. This (rapid) development was induced by Moore's Law that boosted Microelectronics integrated circuits technology. Moore's Law predicted the device dimensions reductions from micro (um) device to deep submicron (nm) devices. However, due to short channel effects induced by the drastic device shrinking, several corrections have to be introduced to maintain this development. The first introduced corrections were called 'engineered devices' and consisted on physical and technological engineering in the basic element (transistor) parts that are the drain, source, channel, substrate and gate. The next step was the introduction of SOI technology which started the layer by layer technology.

SOI engineering initiated the double and later, the Multigate MOSFET which led to the FinFET and later on the GAAFET. These two last devices where designed based on advanced SOI technology, however they could not succeed until the 3D technology was introduced. This technology allowed horizontal and vertical device engineering. Advanced lithography and photolithography are required for implementing devices that are really 3D devices.

In addition to the nanofabrication technology, this talk will describe the design and fabrication of a FinFET and a GAAFET as shown below. 3D technology is still under investigation as it showed some drawbacks in ULSI integrated circuit design.

In any case 3D CMOS or non conventional CMOS has recently reached nodes of 5 and 3nm using respectively FinFETs and GAAFETs.

Nano-Enabled Chemi-Resistive Gas Sensors Based on In_2O_3 And $ZnFe_2O_3$ as VOC Detection Platforms: Effects of Cr-Doping

Gugu Mhlongo*, Murendeni Nemufulwi, Mosima Kgomo
Council for Scientific and Industrial Research (South Africa)
* gmhlongo@csir.co.za

Abstract ID #NN-0730

The development of semiconductor metal oxide (SMO) based chemi-resistive gas sensors have a rich history of about 50 years amongst other types of gas sensors hence they find major applications in various sectors including detection of food adulteration, environmental pollution, human diseases, flammable gases etc. In_2O_3, FeO_2O_4 based-sensors are among the most widely investigated SMOs due to their stability, high catalytic activity, and gas sensitivity, giving them the potential to detect VOCs accurately. However, challenges such as high operating temperatures and selectivity still hinder their practical applicability. To overcome these challenges, previous studies have used high-catalytic metals and SMOs to load on their SMO surface and create heterojunctions [1], [2]. On another note, studies have demonstrated that addition of suitable amount of transition metals into In_2O_3 and $ZnFe_2O_4$ as dopant cations can improve their gas sensing capabilities by providing high content of chemisorbed oxygen ions and oxygen defects/vacancies as these defects serve as adsorption sites for oxygen species, thereby inducing the interaction of target gas molecules and sensing layer [3].

Herein, novel approaches to produce nano-enabled SMO chemi-resistive sensors based on fibrous In_2O_3 and FeO_2O_4 as VOCs sensing platforms have been developed. Numerous characterization techniques have been employed to acquire detailed information pertaining to their structural, morphological, surface defects and textural properties. A comparison of the gas sensing performance findings of the pure 0.5, 1, 1.5 mol% Cr-doped In_2O_3 and FeO_2O_4 nanofibres at different Cr-doping levels revealed that all Cr-doped sensors presented a high response and selectivity towards 50 and 90 ppm Ethanol and Acetone at 80 and 90 ℃, respectively with 1 mol% Cr-doped sensors displaying the highest response values than the rest of the sensors. Furthermore, the response/recovery times of the 1 mol% Cr-doped In_2O_3 and FeO_2O_4 nanofibres were 41/43 s and 45/179 s towards 50 and 90 ppm of Ethanol and Acetone while the minimum detection limit values were 2.19 and 5.1 ppm, respectively. With such rapid response kinetics and a low detection limit, Cr-doped sensors can be a promising active sensing layer for monitoring Ethanol and Acetone in real environments.

ACKNOWLEDGMENTS

This study was supported financially by the Council for Scientific and Industrial Research (Project No. HCARD03) located in South Africa.

PEI-ZIF-8 Overlayer Filter to Enhance the Selectivity of Amine Functionalized Nb_2CT_x Sensor Towards NO_2 Gas at Room Temperature

Naveen Kumar Arkoti*, Kaushik Pal
Indian Institute of Technology Roorkee (India)
* akumar3@nt.iitr.ac.in

Abstract ID #NN-0747

In recent times, the need for the sensitive and selective identification of harmful gases and volatile organic compounds (VOCs) has grown in the areas of clinical, industrial systems monitoring, pollution management and food safety testing applications [1]. Along with other harmful gases, including carbon monoxide (CO), sulfur dioxide (SO_2), ammonia (NH_3), carbon dioxide (CO_2); nitrogen dioxide (NO_2) is one of the main pollutants. Acid showers and ozone depletion are brought on by NO_2, a combustible, colorless gas generated by industrial processes and automobile exhaust [2]. Due to its high sensitivity, selectivity, ease of manufacturing, relatively inexpensive, reduced energy consumption, and low working temperatures, chemiresistive-type sensors are being employed more frequently than conductometric, catalytic, calorimetric, and potentiometric type sensors for detecting such pollutants [3].

A significant issue that restricts their potential applications is the low selectivity of the majority of present chemical sensors. As a NO_2 sensing material in this work, APTES functionalized Nb2CTx MXene is employed [4]. Due to its solubility (imide, isopropylidene, and ether groups on PEI) and diffusion (porousness), Polyetherimide (PEI) integrated with the Zeolitic imidazole framework (ZIF-8) with varied loading (mixed matrix membrane, MMM) is utilised as a selective gas separation membrane [5]. The MMM was selective to NO_2 gas as ZIF-8 is selective towards NO_2 gas, and PEI is resistant to substances like hydrocarbons, alcohols, and halogenated solvents. The PEI-ZIF-8 filter did not significantly alter the sensing response, as evidenced by the 1.6% difference in gas sensing response at 25 ppm NO_2 with and without the filter. ZIF-8 is hydrophobic, hence the Nb_2CT_x-APTES sensor demonstrated greater stability at higher relative humidity (RH) settings. These findings suggest that fabricated sensors can detect NO_2 gas at varying concentrations for environmental and human safety.

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2D Material Based Sensors

Georg Duesberg*
University of the Bundeswehr Munich (Germany)
* duesberg@unibw.de

Abstract ID #NN-0753

Two-dimensional materials such as graphene or transition metal dichalcogenides (TMDs) are intensively investigated for future applications in electronics and sensing. Graphene is highly attractive for chemiresistive gas- and bio-sensors due to its all-surface nature and compatibility with physiological environment. However, strategies for the successful functionalization to yield selectivity are still in infancy, in particular because of detrimental polymeric residues on 2D material surfaces. This will be discusses in the light of TOF-SIMS investigations on polymeric residues. Progress in non-covalent functionalisation of graphene for reliable sensing of small biomarkers will be presented.

As for TMDs, thickness dependent electronic and optical properties such metal-to-semiconductor transitions and high mobilities have moved the group 10 (Pt/Pd) TMDs or Nobel Metal Dichalcogenides (NMDs) to the center of attention. These layered materials have shown high potential for NEMS, optoelectronic devices and chemical sensors. [1] Catalyst free scalable synthesis of polycrystalline of a number of TMDs, in particular PtSe2, is presented in this talk. [2] The direct growth on allows the processing of the layers without mechanical transfer and even deposition on structured substrates [3]. The low temperature synthesis allows the back end of line (BEOL) integration compatible with silicon technology. In this regard, examples for high performance chemical sensors, [1] IR-photodetectors [4] and MEMS [5] devices with $PtSe_2$ will be presented. The composition and morphology of the grown films are investigated by several characterization techniques including Raman spectroscopy, SPM and X-ray photoelectron spectroscopy. Challenges in the understanding of the structure-property relationship of polycrystalline PtSe2 films are discussed.

ACKNOWLEDGMENTS

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No. 881603 (Graphene Flagship Core 3) and No. 101046693 (SSLiP). Further, this project was supported with funds from the German Federal Ministry for Education and Research (BMBF) for project NobelNemS 16ES1121. We thank dtec.bw—Digitalization and Technology Research Center of the Bundeswehr for support [project VITAL-SENSE]. detec.bw is funded by the European Union—NextGenerationEU.

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Pristine and Modified Ga_2O_3 Nanostructure-Based Gas Sensors for Environment and Food Safety

Nyepudzai Charsline Gatsi[1,*], Gugu Mhlongo[2], Nosipho Moloto[3], Rudolph Marthinus Erasmus[4], Odireleng Martin Ntwaeaborwa[5]

[1] *University of the Witwatersrand, Johannesburg. (South Africa)*
[2] *Council for Scientific and Industrial Research (South Africa)*
[3] *School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa. (South Africa)*
[4] *School of Physics and Microscopy and Microanalysis Unit, University of the Witwatersrand, Johannesburg, South Africa. (South Africa)*
[5] *School of Physics, University of the Witwatersrand, Johannesburg, South Africa. (South Africa)*
* nataliya.berezovska@knu.ua

Abstract ID #NN-0798

The release of toxic gases from modern industries seriously threatens the environment's and human's safety [1,2]. Many researchers are therefore committed to developing inexpensive and effective sensors for detecting and monitoring such gases using semiconductor metal oxide (SMO) nanostructures [3]. In this work, a series of studies were conducted to investigate the gas sensing performance of unmodified and noble-metal-modified Ga_2O_3 nanorods prepared using a microwave-assisted hydrothermal method followed by heat treatment. Variation in the heat-treatment temperature induced controlled polymorphism, morphology, and structural defects in Ga_2O_3. The gas sensing measurements revealed a highly selective response, fast response (45s)/recovery (42s) times, and low detection limit of 0.61 ppm towards CO for the β-Ga_2O_3 sensor at a working temperature of 165 ℃. The β-Ga_2O_3 outperformed the α-Ga_2O_3 and α/β-Ga_2O_3 polymorphs due to more active surface sites offered by the high surface area and controlled donor and acceptor defects such as VGa and VO, respectively, for improved surface-target gas interaction. The decoration of β-Ga_2O_3 nanorods surfaces by 1mol% of noble-Ag nanoparticles demonstrated an optimum response coupled with a fast response/recovery time of 38/60 s towards ethylene gas at a lower working temperature of 140 °C. DFT calculations and experimental characterizations revealed that high ethylene sensing benefited several factors including higher adsorption energy of ethylene compared to other target gases, sensitization and catalytic effects of surface plasmonic Ag metals, high surface area and high concentration of defects related to VO and VGa thus offering more active sites for surface-gas interaction. This work demonstrates the potential CO and ethylene sensing capabilities by unmodified β-Ga_2O_3 and 1mol%Ag-modified β-Ga_2O_3, respectively. Ethylene detection is important in food safety–quality monitoring and control in the fruit supply chains [4].

ACKNOWLEDGMENTS

The authors would like to acknowledge financial support from OWSD and Sida (Swedish International Development Cooperation Agency), the National Research Foundation (NRF), and the Council for Scientific and Industrial Research (CSIR).

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Application of Graphene-Based Nanostructures Enabling Signal Enhancement for Electrochemical Detection of Progesterone Hormone

Disha disha[1,2], Poonam Kumari[2,*], Raj Rani[2], Manoj Kumar Nayak[3]
[1] *CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C Chandigarh (India)*
[2] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India (India)*
[3] *AcSIR, CSIR-CSIO,Chandigarh (India)*
* p.bangarwa77@gmail.com

Abstract ID #NN-0802

In the past years, numerous reports have documented the endocrine disrupting activity of steroid hormones including progesterone, a potent lipophilic compound which is essential for the diagnosis of various reproductive health disorders and hormonal imbalance [1-3]. Owing to the admirable physio-chemical characteristics, graphene and its functional nanocomposites have garnered a considerable attention in the domains of electrochemical sensing. Herein, the proposed work presented the usage of Magnetic nanocomposites of graphene oxide (MGO) as an electrode casting material for constructing immuno-sensing platform for progesterone hormone. MGO decorated screen printed electrodes were further implemented as bio-receptors immobilization matrix due to its enhanced electrochemical response as well as the availability of plenty of active groups for binding antibodies.

The electrochemical performance was investigated with both Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV) techniques for effective detection and analysis. Under optimum experimental parameters, the present method displayed excellent repeatability, selectivity, fine stability and a good linearity from 0.01 pM to 1000 nM with low detection limits i.e. 0.15 pM (with DPV) and 0.17 pM (with CV). Subsequently, the developed biosensor was applied in real sample analysis practically with spiked water samples and exhibited satisfactory recovery performance. Furthermore, the morphological and structural properties of MGO were studied through various characterization methods such as FE-SEM, FTIR, XRD, and RAMAN. Application of two electrochemical techniques (CV and DPV) in the study has significantly improved the sensor's performance as cost effective as well as reliable detection approach. The stated work successfully signifies the potential applications of detecting progesterone in biological matrices such as saliva, blood serum and urine.

ACKNOWLEDGMENTS

CSIR-Central Scientific Instruments Organization (CSIO), Chandigarh, India, supported this work. The authors express their gratitude to the UGC and CSIR-CSIO.

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Hydrogen Sensing Characteristics of TiO_2 Thin Films Grown by Atomic Layer Depositon Using TTIP Precursor with H_2O vs. O_3 reactants

Boris Hudec[1,*], Tomáš Ščepka[1], Matej Horský[1], Peter Nádaždy[1], Iuliia Vetrova[1], Martin Predanocy[2], Pavol NEMEC[2], Róbert Andok[2], Michal Patrnčiak[3], Tomáš Plecenik[4]

[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[2] *Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia (Slovakia)*

[3] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava (Slovakia)*

[4] *Faculty of Mathematics, Physics and Informatics, Comenius University Bratislava, Mlynska dolina F2, Bratislava 84248 (Slovakia)*

* boris.hudec@savba.sk

Abstract ID #NN-0838

It has been shown that passive chemiresistive thin film hydrogen gas sensors fabricated using physical vapour deposited (PVD) sandwich of $Pt/TiO_2/Pt$ can provide sufficient sensitivity even when operating at room temperature [1,2]. It was also shown that thickness, microstructure and crystallinity of TiO_2 have strong effect on the hydrogen sensing characteristics of these thin film sensors [3].

In this work, we have fabricated TiO_2 thin films in $Pt/TiO_2/Pt$ hydrogen sensing structures using atomic layer deposition (ALD). Using ALD, conformal, pinhole-free and crystalline TiO_2 films can be obtained even for thicknesses of 10 and 20 nm, at a moderate temperature of 300 °C [4], which were the conditions used also in this study. In one of our previous works we have shown that ALD TiO_2 process using TTIP precursor and O_3 reactant produces films with smaller grains as compared to the process with $TiCl_4$ precursor and H_2O reactant, which produced larger grains [5]. As the crystallinity and microstructure are key properties for the hydrogen sensing characteristics of TiO_2, in this study we have compared 10 and 20 nm thick films made using TTIP with two different reactants, namely H_2O and O_3. The resulting hydrogen sensing characteristics of these films are discussed in regards to the microstructure of these films, characterized using scanning electron microscopy (SEM), atomic force microscopy (AFM) and X-ray diffraction (XRD). Finally, we discuss the suitability of the $Pt/TiO_2/TiN$ --diode structure [4] with TiN bottom electrode for the hydrogen sensors in comparison to more commonly used $Pt/TiO_2/Pt$ structure.

ACKNOWLEDGMENTS

This work was supported by the Operational Program Integrated Infrastructure for the project: New fabrication technology of sensors, detectors and memristors for intelligent microelectronics in the 21st century, ITMS project code 313011BVN5, co-financed by the European Regional Development Fund (ERDF) (0.5). This work was supported by the Slovak Research and Development Agency under the contract No. APVV-21-0053, an project VEGA 2/0099/22.

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Superconducting Nanowire Devices: Particle Detectors and Electronics

Tomas Polakovic*, Timothy Draher, Yi Li, Valentine Novosad
Argonne National Laboratory (United States)
* tpolakovic@anl.gov

Abstract ID #NN-0839

Superconducting nanowire single-photon detectors have become a prominent technology in the fields of quantum optics and quantum communication, primarily due to their low timing jitter and ability to detect individual low-energy photons with exceptional quantum efficiencies. However, the literature often underrepresents other advantageous characteristics, such as high detection rates, compatibility with cryogenic and high magnetic field environments, and the efficient detection of charged particles. This underrepresentation may unintentionally limit interest from other disciplines that could benefit from this technology.

In this presentation, I will discuss the advancements made in applications related to particle physics experiments, microelectronics, and hybrid quantum systems. I will emphasize the use of novel materials and designs that deviate from conventional approaches in single-photon counting applications. Additionally, I will address the unique challenges faced by these systems and applications, fostering further exploration and development in these areas.

ACKNOWLEDGMENTS

This work was supported by the U. S. Department of Energy (DOE), Office of Science, Offices of Nuclear Physics, Basic Energy Sciences, Materials Sciences and Engineering Division under Contract #DE-AC02-06CH11357.

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Vertical Heterostructure TiO_2 Gas Sensor for Low-Temperature Detection of H_2 Via Maskless UV Photolithography

Pavol NEMEC*, Martin Predanocy, Róbert Andok, Jaroslava Škriniarová, Jaromír Klarák
Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia (Slovakia)
* pavol.nemec@savba.sk

Abstract ID #NN-0851

The change in the conductivity properties of titanium dioxide (TiO_2) upon its exposure to hydrogen (H_2) predisposes this thin-film material to its use as an active layer in gas sensors. There are various ways to modify the properties of a TiO_2 thin layer with the main goal of increasing its sensitivity to test gases. Modification of TiO2 by annealing changes its surface and structural properties while these changes ensure its increased sensitivity to H_2 [1].

Maskless photolithography [2] is a modern, fast and cheap method of optical lithography applicable to the production of microelectronic devices. Moreover, it allows changing the design of ad hoc structures making it possible to create complex pre-designed patterns with high accuracy that can be changed depending on the results of previous measurements or simulations. The possibility of variability in the production of gas sensor prototypes gives a powerful tool to achieve high-sensitivity gas sensors that detect very low concentrations of the test gas at low operating temperatures [3].

In our work, Si was used as substrate material, and 300nm SiO_2 as insulating material on top. The vertical structure of the sensor consists of a lower Pt IDE (interdigital electrodes) contact of 30 nm, an active TiO_2 layer of 100 nm and an upper Pt IDE electrode.

A thin TiO_2 film was deposited at room temperature by DC reactive magnetron sputtering from a Ti target in an O_2-Ar gas mixture at a working pressure of 0.095 Pa and sputtering power of 70 W. The relative partial pressure of O_2 was 25%. Improvement of the structural and electrical properties of the Pt/TiO_2/Pt heterostructure was achieved by annealing in technical air at temperatures of 400, 500 and 600°C, respectively. It was found that large grains are formed at annealing temperatures higher than 600°C when hydrogen diffusion into the TiO2 volume is reduced.

The measurement of properties such as dynamic response, temperature dependence of the gas sensor for in such way prepared samples took place in technical gas with different concentrations of H_2. The samples were contacted using the two-probe method and placed in a chamber with a temperature-controlled table and gas supply. LTS420 chamber was used with temperature changing from 25°C to 300°C. For resistance measurements Agilent 34410A (precision source/measure unit) was used.

We have modified the shape and structure of the Pt/TiO_2/Pt heterostructure by changing the design proposal using non-contact photolithography. We compared the increase in sensitivity, selectivity, dynamic response and temperature dependence of different gas sensor designs. The possibility of immediate changes using maskless photolithography in the design can simplify and accelerate the development process of the TiO_2-based gas sensor. The resulting measured characteristics of the heterostructure were compared with each other with a focus on the detection of the lowest H_2 concentrations at room temperature.

ACKNOWLEDGMENTS

This work was financially supported by the Scientific Grant Agency of the Ministry of Education of Slovak Republic and the Slovak Academy of Sciences with projects VEGA No. 2/0099/22, 1/0789/21. The authors would like to thank Ivan Hotový and for his assistance in the deposition of SiO_2 and TiO_2 layers and for his help and fruitful scientific discussions.

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Carbon Nanodots for the Electrochemical Biosensing of Thyroxine Hormone

Mradula Mradula*
CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C Chandigarh (India)
* mradula992@gmail.com

Abstract ID #NN-0860

Thyroid is the most common condition worldwide and many affected populations are unaware of their condition [1]. An electrochemical (ECL) immunosensor is proposed for the detection of thyroxine hormone. The amine functionalized carbon quantum dots (NCQDs) are synthesized from the precursor citric acid and ammonia via the hydrothermal route [2]. These carbon dots were functionalized with anti-TNT antibody via EDC-NHS cross-linking chemistry and used as probe for the quantitative and qualitative analysis of thyroxine hormone. The electrochemical characterization and thyroxine sensing was done by cyclic voltammetry (CV) and differential pulse voltammetry (DPV) techniques. The immunosensor possessed a dynamic linear range (10–104 pM) with a detection limit in the picomolar range. The proposed immunosensor exhibits good selectivity, sensitivity, repeatability, and stability, therefore, can be explored further as a promising platform for the rapid and direct analysis of thyroxine in serum samples. The designed probe is also used for the fluorescent sensing of thyroxine hormone and other analytes.

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Development of Fluorescent Silver Nanocluster Incorporated Hydrogel Platform for Detection of Antioxidants

Rocky Raj[1,*], Abhay Sachdev[2], Sunita Mishra[3]
[1] *AcSIR, CSIR-CSIO,Chandigarh (India)*
[2] *Central Scientific Instruments Organisation, Chandigarh, India (India)*
[3] *Academy of Scientific and Innovative Research (India)*
* rockyraj.latyal92@gmail.com

Abstract ID #NN-0861

Antioxidant determination has become one of the most common analytical procedure in medical, pharmaceutical and food industries. In this study, water soluble fluorescent silver nanoclusters with blue-green emission (ʎexc=350nm; ʎem=470nm), were synthesized and investigated for their potential to recognize antioxidants. Using ascorbic acid as a model antioxidant, a simple one step visual colorimetric and fluorometric assay was developed for antioxidant determination. The developed assay demonstrated wide dynamic detection range from 10-10^4 µM and linear detection range from 10^2-10^4 µM for ascorbic acid, under optimal conditions. The sensing mechanism behind the detection was observed to be the combination of dynamic and static quenching processes. The silver nanoclusters were further incorporated in a hydrogel platform for solid state detection. The developed assay showed good accuracy when employed for detection of antioxidant activity in ascorbic acid spiked green tea samples in comparison to standard antioxidant assays.

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Influence of Hydrogen Ions on the Properties of the Plasmon Resonance Sensor

Taras Vasyliev[1,*], Anatoliy Vasiljev[1], Viktor Kryvytskyi[1], Roman Zhelezniak[1], Tamara Doroshenko[2]
[1] *National Taras Shevchenko University of Kyiv (Ukraine)*
[2] *State Scientific - Production Association of Optics, Optoelectronics and Laser Technology (Ukraine)*
* taras.a.vasiliev@gmail.com

Abstract ID #NN-0862

The present studies were devoted to the effect of hydrogen ions on the surface plasmon resonance (SPR) sensor. To create a flow of hydrogen ions, electrolysis in an aqueous solution of H2SO4 was used. The properties of the SPR sensor mainly depend on the properties of the surface layer of the gold film. Therefore, we chose the pulse regime of electrolysis for the experiments. The lasting of the electrolysis current pulse was 2s. The current during the pulse was 5 μA. Current pulses were repeated every minute. Therefore, during the pulse, the surface of the SPR sensor received ions, and hydrogen saturated the gold film. Degassing occurred during the 58s between pulses. The SPR spectrum of the treated sensor was experimentally studied. After the effect of 15 pulses on the sensor, the SPR curve for each tasted sample shifted to the region of larger angles. The width of each SPR curve increased. The amplitude of resonant absorption of light decreased significantly.

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Frequency-Tunable High-Q Superconducting Resonator via Nonlinear Kinetic Inductance Control with Flux Coupling

Juliang Li[1], Pete Barry[2], Tom Cecil[1], Marharyta Lisovenko[1], Volodymyr Yefremenko[1], Gensheng Wang[1], Serhii Kruhlov[3,*], Goran Karapetrov[3], Clarence Chang[1]

[1] *Argonne National Laboratory (United States)*
[2] *Cardiff University (United Kingdom)*
[3] *Drexel University (United States)*

* sk3997@drexel.edu

Abstract ID #NN-0863

In this work we present the design of the kinetic inductance-based frequency-tunable high-Q superconducting resonator with flux coupling capability. The resonator was fabricated with thin aluminum film and consisted of lumped LC elements. Superconducting loop was formed with two inductors symmetrically placed on the left and right sides of an interdigital capacitor with capacitor ends. Magnetic flux generated by a DC current on the RF readout line excites a screening current in the superconducting loop and resonant frequency is tuned nonlinear kinetic inductance in the two inductors is function of the exited DC. A continuous frequency tuning of 200 MHz is achieved for a 2.7 GHz resonator with a maximum current of 8mA while the 'wireless' DC bias ensures the resonator maintains its high Q. We demonstrated flux coupling capability of the resonator with 3 wave mixing process by parametric pumping on the nonlinear kinetic inductance through the readout line. This flux coupling capability also enables frequency upconverter and we evaluated this by applying a 10kHz modulation signal on DC bias line. The integrity and simplicity of the design greatly eases the fabrication process and enables large array multiplexing and on chip compatibility. Its immediate application is hybrid superconducting system where frequency matching is required. It also has the potential application of parametric amplifiers and magnetometer that working at Kelvin temperatures.

Advances in Planar-Hall Magnetoresistive Sensors and their Robust Applications

CheolGi Kim*
Department of Emerging Materials Science, DGIST, Daegu, 42988 (Republic of Korea)
* cgkim@dgist.ac.kr

Abstract ID #NN-0877

Rapid advancements in micro- and nano-technology have led to the widespread use of spintronic sensors in both recording and non-recording applications. Among these sensors, the state-of-the-art planar-Hall magnetoresistive (PHMR) sensors exhibit high sensitivities and ultra-low field detectivities, making them well-suited for use in smart sensing applications across a range of industries like as in the fields of internet of things, mobile devices, space technology, aeronautics, magnetic flux leakage, the environment, and healthcare [1, 2]. This study will first review the specific features of PHMR sensors, including their thermal stability and tunable field sensitivity. Here, thermal drift is very low about 0.02 Ω/°C, compared with that of other MR sensors ~ 10 Ω/°C. Another feature is the tunable field sensitivity by adjusting exchange coupling field using the nonmagnetic Cu layer between NiFe and IrMn, and the ring number, from ~ a few μV/Oe for cross type to 2 mV/Oe for 7 ring sensor [3].

We will then introduce some of the robust applications of PHMR sensors, such as on-chip magnetometries integrated in micro-fluidic channels for biochip and susceptometer, industrial and magnetic synapse [4]. These applications showcase the remarkable sensitivity of PHMR sensors, with a maximum magnetic moment resolution of ~ 10-14 emu in dried conditions, which is 104 orders better than conventional SQUID magnetometers [5]. With their ability to be customized and miniaturized, as well as their cost-effective nature, PHMR sensors are uniquely competitive and offer significant potential for mass production and non-recording industrial applications.

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Ultrasensitive p-n Heterostructured Thin Film Gas Sensors for N_2O Gas Detection

Amanzhol Turlybekuly[1,*], Yernar Shynybekov[2], Almagul Mentbayeva[2], Baktiyar Soltabayev[1]
[1] *National Laboratory Astana, Nazarbayev University, Astana (Kazakhstan)*
[2] *School of Engineering and Digital Sciences, Nazarbayev University, Nur-Sultan (Kazakhstan)*
* amanzhol.turlybekuly@nu.edu.kz

Abstract ID #NN-0901

Nitrous oxide (N_2O), a perilous gas widely employed for its anesthetic properties during surgeries, is discharged into the atmosphere untreated. Despite its relatively low presence in the air, its impact on the greenhouse effect is disproportionately potent, possessing a warming coefficient approximately 300 times greater than that of CO_2 [1]. Limited research has been dedicated to the advancement of sensors capable of detecting N_2O gas, particularly at room temperature (RT) and extremely low concentrations [2, 3].

In this investigation, we engineered an exquisitely sensitive gas-detecting apparatus designed for operation at RT. This innovation relies on CuO/TiO_2 heterojunctioned nanointerfaces created through a scalable reactive magnetron sputtering technique utilizing glancing angle deposition. The CuO/TiO_2 heterojunctioned nanointerfaces exhibited a N_2O gas sensitivity around twice that of a standalone TiO_2 layer. Notably, the device boasts an exceptional detection threshold of 50 parts per billion (ppb) at RT, while also displaying rapid response and recovery times of approximately 36 seconds and 50 seconds, respectively.

This heightened gas-sensing sensitivity is achieved through meticulous control over the nanoarchitecture, ensuring that the nanorods-like structure closely aligns with doubled Debye lengths [4, 5], measuring roughly 70-80 nanometers. The strategic design of this nanoarchitecture establishes a versatile platform for various gas sensing devices, effectively harnessing an array of p-n heterojunction nanorods with simplicity and efficacy. Rigorous statistical analyses affirm the robustness and reproducibility of the collected data.

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TRACK 10

“NANOMATERIALS FOR ENERGY & ENVIRONMENT”

Efficient Adsorbent Graphene Oxide Nanoparticles from Agricultural Waste for DR-81 Decontamination

Eslam Salama*, Mona Ossman
Environment and Natural Materials Research Institute (ENMRI), City of Scientific Research and Technological Applications (SRTA-City), New Borg El-Arab City, Alexandria 21934, Egypt (Egypt)

* esalama@srtacity.sci.eg

Abstract ID #NEE-463

In this investigation, we presented a cost-effective method for producing high-content carbon material like graphene oxide (GO) through the gasification of agricultural waste such as palm leaves. GO was further synthesized from the produced carbon material using a muffle furnace at 800°C for 3 h. The synthesized material was characterized using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), field emission transmission electron microscopy (FETEM), thermal gravimetrical analysis (TGA), and Brunauer-Emmett-Teller (BET) surface area analysis. The prepared nanomaterial was employed as an efficient adsorbent for direct red 81 (DR-81) dye from wastewater. Several processing variables, including pH, contact time, and dosage were studied to examine the decontamination of DR-81 anionic dye onto the fabricated GO. The optimal dosage from the synthesized GO for DR-81 decontamination was 1.0 g/L at pH=7 after 30 min. The maximum sorption capacity of the prepared GO toward the DR-81 was 132.14 mg/g at pH 7.0 and 25°C. These promising findings supported the use of synthesized GO as a superior adsorbent material for DR-81 decontamination from wastewater.

Improvement of Specific Capacity of Lithium Iron Phosphate Battery By Increasing The Surface Area And Electrical Conductivity of Cathode Electrode Using Graphene Foam

Piyaporn Surinlert[1*], Akkawat Ruammaitree[2]
[1] *Thammasat University (Thailand)*
[2] *Department of Physics, Faculty of Science and Technology, Thammasat University (Thailand)*

* piyaporn.latte@gmail.com

Abstract ID #NEE-467

Lithium iron phosphate (LFP) is widely used as an active material in a cathode electrode for lithium-ion batteries (LIBs). LFP has many remarkable properties such as high working voltage and excellent thermal stability. However, it suffers with slow ion diffusion and low electrical conductivity. Graphene foam has many outstanding properties such as large surface area and great electrical conductivity. These properties are suitable for improving the cathode electrode. In this work, the graphene foam was synthesized by chemical vapor deposition. The cathode electrode was prepared by dropping the LFP on the graphene foam. We found that the specific capacity of battery which contained the LFP between the anode and the graphene foam (LFP/GF) was 23.1 mAh/g at 3C, while the specific capacity of battery which contained the graphene foam between the anode and the LFP (GF/LFP) was 112.6 mAh/g at 3C. Specific capacity of GF/LFP was higher than that of LFP/GF at high current density due to the high ion transfer rate which arises from graphene foam.

ACKNOWLEDGMENTS

This work was supported by the Thailand Science Research and Innovation Fundamental Fund fiscal year 2023, and Thammasat University Research Fund, Contract No. TUFT 7/2564, and Thammasat University Research Unit in Synthesis and Applications of Graphene.

Development of Fenton-Like Process Using Magnetic Iron Oxide Nanoparticles to Decolorize and Degrade Disperse Azo Dye by Photocatalysis

Pravinkumar Ranchhodbhai Dudhagara*, Sunil Bhavsar
Veer Narmad South Gujarat University (India)

* dudhagarapr@gmail.com

Abstract ID #NEE-469

Textile industry effluents contain several hazardous substances, such as dye-containing effluents pose environmental and aesthetic challenges. Presently, the microbial-based remediation process is in use. However, the microbial process is affected by effluent characteristics and environmental parameters. Using nanotechnology-based methods to overcome the limitations of the microbial remediation process is a new emerging trend. For large-scale contaminated areas, nanoremediation may result in more cost-effective and time-efficient in situ cleanup techniques.

To remove scattered dyes from industrial effluents, this study employed readily available nanoadsorbents, the ferrous ferric oxide (Fe_3O_4) nanoparticles, to investigate their effectiveness. The ferrous ferric oxide nanoparticles were prepared by a chemical co-precipitation method. They had 26.93 emug-1 magnetizations with sizes smaller than 20 nm, highly purified with cubic spinel crystallite structure. The catalytic activity of iron oxide depended on the dose, photocatalytic enhancer, i.e., H_2O_2 or oxalic acid level, pH of the reaction medium, and dye concentration. We optimized the Fenton-like reaction using 1.0 g/L of ferrous ferric oxide nanoparticles and 60 mM oxalic acid at pH 7.0, using 60 ppm dye concentration. Iron oxides act as photocatalysts, and oxalic acid generates electron-hole pairs. Consequently, a higher amount of super radicals cause the rapid degradation of dye. LC-MS analysis revealed the ferrous ferric oxide nanoparticles decolourized and destroyed disperse red 277 in 180 minutes under visible light. Hence complete de-mineralization is observed using a photo Fenton-like reaction within 3 hours under visible light. It is suggested that the high-capacity, easy-to-separate next-generation adsorption systems are suitable for industrial-scale use. Ferrous ferric oxide nanoparticles with increased adsorption and magnetic properties could be utilized to address environmental issues. The research showed a customized Fenton-like reaction that photocatalyzes textile dye using non-hazardous oxalic acid instead of H_2O_2. Industrial dye removal in 3 hours is possible.

In summary, ferrous ferric oxide nanoparticles' enhanced adsorption and magnetic properties could solve many environmental issues. Ferrous ferric oxide nanoparticles may enable the creation of high-absorption, efficient separation adsorption nanomaterials. Ferrous ferric oxide nanoparticles' photochemical and magnetic properties enable innovative applications in more efficient and cost-effective environmental remediation than conventional technologies. Nanoadsorbents could meet industrial effluent treatment needs economically.

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Superlattice-based Plasmonic Catalysis for Efficient Nitrogen Reduction Reaction at Ambient Conditions

Siew Kheng Boong*, Hiang Kwee Lee
Nanyang Technological University (Singapore)

* siewkhen001@e.ntu.edu.sg

Abstract ID #NEE- 470

Plasmonic metal nanoparticles promise efficient and greener ammonia synthesis under mild/ambient conditions. Due to the use of metallic nanoparticles, plasmonic catalyst is able to concentrate light energy directly on catalytic surfaces through the localized surface plasmon resonance (LSPR) effect. This unique light-matter interaction spans across the UV-vis-IR regions, notably allowing facile reaction activation via intriguing plasmonic phenomena such as hot electron transfer and field polarization effects. However, current plasmonic catalysis design is limited by the need of co-catalysts and poor performances due to weak electromagnetic field enhancement. Here, we organize anisotropic plasmonic nanoparticles into a two-dimensional superlattice with dense electromagnetic hotspots to boost ambient nitrogen-to-ammonia photoconversion without needing co-catalyst. By assembling Ag octahedra into a square superlattice to concentrate light, the ammonia formation is enhanced by ≈15-fold and 4-fold over hexagonal superlattice and disorganized array, respectively. Our unique superlattice-based plasmonic catalysts achieve superior ammonia formation rate and apparent quantum yield up to ≈15-fold and 103-fold, respectively, better than traditional designs. Systematic investigations into structure-to-plasmonic-to-catalytic properties affirm the generation of intense plasmonic hotspots is the fundamental basis to create energetically hot electrons on the catalyst for nitrogen reduction. Our work offers valuable insights to design electromagnetically hot plasmonic catalysts for diverse chemical and energy applications.

ACKNOWLEDGMENTS

We thank the funding supports from Singapore Ministry of Education (RS13/20 and RG4/21), Agency for Science, Technology and Research, Singapore (A*STAR, A2084c0158), Center of Hydrogen Innovation, National University of Singapore (CHI-P2022-05), and Nanyang Technological University start-up grants. The research was conducted as a part of NICES (NTU-IMRE Chemistry Lab for Eco Sustainability; REQ0275931), a joint research initiative between Nanyang Technological University (NTU) and Institute of Materials Research and Engineering (IMRE) from Agency for Science, Technology and Research (A*STAR).

Hectorite Nanoparticle as a Shear-thixotropic Plugging Agent in Water-based Drilling Fluids

Chunping Guo, Guancheng Jiang*
China University of Petroleum-Beijing (China)

* 1799947178@qq.com

Abstract ID #NEE-472

In this research, we demonstrated an artificial nano-clay particles, Hectorite, as a shear-thixotropic plugging agent for Lost Circulation Control in water-based drilling fluids. We compared the shear-thixotropic properties of hectorite and other nano particles, as well as the inorganic plugging properties of hectorite and calcium carbonate in water-based drilling fluids. In stress-shear rate test, the rheological models of several nano particles were consistent with H-B model, but Hectorite had the highest R2 value of 97%. Hectorite had an intermediate n value with good shear thinning behavior, which was also confirmed by the viscosity-shear rate test, the largest k value with the best thickening properties, and a higher yield point of 6.44Pa with better suspension performance. In thixotropic test, the recovered G' of 1% Hectorite in the three interval thixotropy test (3ITT) performs better than other nano-clay particles, and its thixotropic area has the biggest value at 3089Pa/s. In particle plugging tests (PPT), 0.8% Hectorite (6.8 mL) leaked less than 2% calcium carbonate (72.5 mL) in 40–60 mesh quartz sand at 90 °C and 4 MPa after 30 minutes. The flat surface of the Hectorite filter cake was seen in TEM pictures, which helped to explain its effective plugging properties.

ACKNOWLEDGMENTS

National Natural Science Foundation of China (NSFC) 51991361;

National Natural Science Foundation of China (NSFC) 52004297;

Foundation of China University of Petroleum (Beijing) 2462022YJRC005;

Foundation of China University of Petroleum (Beijing) 2462021YXZZ002

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Photocatalysis and Photosensitization Using Atomically Precise Metal Nanoclusters for Solar Energy Harvesting and Conversion

Ye Liu, Yu Wang, Nicola Pinna*
Institut für Chemie and IRIS Adlershof, Humboldt-Universität zu Berlin (Germany)

* nicola.pinna@hu-berlin.de

Abstract ID #NEE-473

Metal nanoclusters (NCs) with atomic precision are a unique family of metal nanomaterials that are readily crystalized into single crystals, representing ideal models to unravel structure-property relationship at atomic level. By tuning the number of metal atoms in the core, the composition and the protecting ligand of metal NCs, their physicochemical properties can be precisely controlled. The strong, broad light absorption ability and the long-lived excited states make metal NCs promising candidates as photosensitizer, and might replace traditional dyes. Their discrete energy levels allow them to prevent charge recombination at the semiconductor by efficiently separate the photoinduced charge carriers. Moreover, these metal NCs themselves can act as active catalysts. In the first part of the talk, we demonstrate the differences of working principle between metal NCs and their particle counterparts in photocatalytic system. The metal NC modified TiO2 catalyst is found to exhibit a fiver times higher performance than TiO2 modified with metal nanoparticles in the photocatalytic H2 production reaction.[1] In the second part, we present the strategy to tune the charge transfer pathways of metal NCs sensitized semiconductors in photoelectrochemical system. While metal NCs serve as catalyst for oxidation reactions when loaded on n-type semiconductor, they serve as catalyst for reduction reactions when loaded on p-type semiconductor.[2] In the last part, we will use Au25 NC as an example to demonstrate how the protecting ligand and the composition of the metal NC influence the overall performance of a NC/semiconductor system in photocatalytic H2 production.[3]

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Carbon Nanotubes Heterojunction With Graphene Like Carbon Nitride for The Enhancement of Electrochemical and Photocatalytic Activity

Tahir Muhmood*
Nanjing Forestry University (China)

* muhmoodtahir@yahoo.com

Abstract ID #NEE-481

This research reported electro-static junctions between carbon nanotubes (CNT) and graphitic carbon nitride (CCN) with enhanced photocatalytic properties. The CNT and CCN formed the CTCN (CNT/CCN) by the electrostatistic driving force under hydrothermal methodology. The materials fabrication was confirmed by using different analyzing techniques such as SEM, TEM, XRD, and FTIR (etc). Also, the photocatalytic ability was studied by the degradation of R-610 under visible light irradiation. The CTCN-1 possess the higher degradation rate 0.0105 min− 1 and higher current density 0.19 μA/cm2 as compare to other, CTCN-2 (0.0088 min− 1, 0.16 μA/cm2), CTCN-3 (0.0065 min− 1, 0.12 μA/cm2) and CCN (0.0035 min− 1, 0.10 μA/cm2). The combining of CNT with CCN in a specific amount reduces the structure defects in graphitic carbon nitride by reducing the charge recombination ability. Ion-trapping experiments showed that superoxide radicals and holes are the most generated and effective photogenerated species to accomplish the degradation of R-610 (rhodamine-610) under visible light irradiation. A junction was created between CCN and CNT under electrostatic force by the hydrothermal methodology. Analysis results indicated that the junctions were created successfully between CCN and CNT. The CTCN-1 shows the best degradation results as compared to the CTCN-2 and CTCN-3, which indicated that only a specific amount of CNT can enhance the catalytic ability, higher quantity decreases the ability due to mustiness in the structure. Almost CTCN-1 completely degraded the R- 610 with a higher rate0.0105 min− 1, as compared to others degradation, 80% (CTCN-2), 55% (CTCN-3), and 30% (CCN), with degradation rate 0.0088 min− 1, 0.0065 min− 1 and 0.0035 min− 1 respectively, in the same interval of time. The blank test also indicated that the R-610 was not degraded due to the sensitization effect. The addition of CNT can suppress the recombination of photogenerated charge carriers (e− , h+), so enhanced the photocatalytic ability of CTCN.

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Polydopamine Modified Graphene Oxide Nanocomposite Membranes for Efficient Dye Removal from Water

Swati Gahlot[1*], Vaibhav Kulshrestha[2], Bijay Prakash Tripathi[3]
[1] *Sardar Vallabhbhai National Institute of Technology (India)*
[2] *CSIR-Central Salt and Marine Chemicals Research Institute Bhavnagar India (India)*
[3] *Indian Institute of Technology Delhi (India)*

* gahlot.swati20@gmail.com

Abstract ID #NEE-487

In recent years, industrialization has caused numerous adverse effects on environment. One of them is the water pollution caused by dyes waste from textile industries. Nanotechnology is playing a significant role in combating environmental issues [1]. Graphene, the most versatile material, has created a prominent place in research in the recent past [2]. Porous structure of Graphene Oxide (GO) laminates enables its use in separation and purification application [3, 4]. Studies demonstrate that micrometer thick graphene oxide membranes are utterly impermeable to gases, liquids while permitting unrestricted permeation of water [5]. Herein we report the synthesis of nanocomposite membranes of Graphene oxide (GO) with polyacrylonitrile (PAN) polymer via phase inversion method for dye removal application. Graphene Oxide has been synthesized via Hummer's method followed by the modification with polydopamine (PDA-GO). Dopamine polymerized to polydopamine (PDA) through oxidative polymerization is helpful in adhering to other surfaces. PAN membrane has been fabricated containing different ratios of PDA-GO(2, 5 and 10wt%) within the matrix. Membranes without PDA coated GO, pure PAN has been prepared for the comparison. Prepared membranes have been examined for water permeation and dye rejection performance. P-PDAGO5(5wt% PDA-GO) membrane shows the best water permeation performance among all prepared membranes. Membranes have been found effective towards Congo red dye rejection.

ACKNOWLEDGMENTS

The authors wish to acknowledge Leibniz-Institut für Polymerforschung, Dresden for funding and instrumental characterization, CSIR- Central Salt and Marine Chemical Research Institute, Bhavnagar, Gujarat and Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat.

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Formation of Nanopores in Anodic Oxidized Aluminium Affected by Carbon Nanodots

Ludmila Ponomarova[1*], Kateryna Kudelko[2], Olexander Dziazko[3], Ludmila Rozhdesvenska[2], Liudmila Kharkova[2]

[1] *Sumy State University (Ukraine)*
[2] *V.Vernadsky Institute of General and Inorganic Chemistry, NAS of Ukraine (Ukraine)*
[3] *Taras Shevchenko National University of Kyiv (Ukraine)*

* l.ponomarova@chem.sumdu.edu.ua

Abstract ID #NEE-506

Among hydrated oxides of multivalent metals, which are used as adsorbents and modifiers of ion exchange resins [1], polymer [2] and inorganic membranes [3], anodic oxidized aluminium (AOA) occupies special position, since it is obtained in a massive form, and characterized by through regular pore structure [4]. As a rule, AOA with nanosized pores can be obtained in aggressive or toxic media, pores, a size of which exceeds 100 nm, are formed in eco-friendly electrolyte (oxalic acid). Earlier we used the additions of graphene oxide (GO) to the solution of oxalic acid in order to decrease pore used as an additions to eco-friendly electrolyte to decrease pore size [5]. Carbon nanodotes (CNDs), synthesis of which requires no aggressive reagents [6], are good candidates as an additions to the electrolyte.

In this work, the problem of reducing size of the AOA pores has been solved by using colloidal CNDs solution added to the solution of oxalic acid. Here the mechanism of CNDs action on the pore formation has been proposed: they are adsorbed on the AOA surface increasing the current density on unshielded regions. The hydrothermal treatment of AOA was found to result in transformation to crystalline modifications of aluminium oxide, such as δ-Al and corundum.

The addition of colloidal CNDs particles to the solution of weak acid allows us to decrease pore size from 75-100 nm down to 20-40 nm similar to [5]. The advantage of CNDs over GO is eco-friendly and fast synthesis. Adsorption isotherm of CNDs on AOA was found to obey Temkin model indicating energetic heterogeneity of surface. Aggregated CNDs nanoparticles are also adsorbed by AOA, as was suggested with a method of dynamic laser scattering. Our results demonstrate a possibility to urposeful control of pore size by regulation of the composition of a mixed electrolyte. Our results give a possibility to obtain nanoporous AOA under eco-friendly conditions.

Moreover, hydrothermal treatment allows us to transform AOA into mechanically durable form. CNDs are not removed from AOA under these conditions. This gives a possibility to consider nanoporous AOA as a membrane with hydrophilic properties, which provide its stability against fouling.

ACKNOWLEDGMENTS

The work was performed within the framework of the project "Development of membranes modified with composites based on polymer with inorganic hydrophylized and antibacterial additions" (program number 0122U001235).

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A Zr-Mof and Conductive Polymer Based Sensitive Electrochemical Detection of Nitrofurantoin Antibiotics In Water

Shalini Singh[1*], Priyanshu Goel[2], Deepanshu Bhatt[2], Umesh Tiwari[3], Akash Deep[4]
[1] *AcSIR, CSIR-CSIO,Chandigarh (India)*
[2] *Academy of Scientific and Innovative Research (India)*
[3] *Central Scientific Instruments Organisation, Chandigarh, India (India)*
[4] *Institute of Nano Science and Technology (India)*

* shalini92.csio@gmail.com

Abstract ID #NEE-514

The illegitimate use and disposal of antibiotics have been turned into a threat to the environment and ecosystem. As a result of this, surveillance of many such antibiotics has been an alarming need to safeguard public health. The different metal-organic frameworks and their composites-based electrochemical sensing platforms have been explored over the decade for the various applications of environmental pollutants such as antibiotics, heavy metals, food toxins and dyes. This work presents the Zirconium metal-organic framework incorporated polythiophene-based sensitive electrochemical detection platform for nitrofurantoin antibiotics residues in water. The electrochemical-based sensing platform was designed on the graphite foil using the drop casting method for Zr MOF followed by Cyclic voltammetry-assisted electrochemical deposition of polythiophene (PTh). The spectroscopic and morphological characterization of the fabricated composite has been performed on FT-IR, UV-Vis, XRD, Raman, and electron microscopy. The developed MOF and polythiophene-based sensing platform is found to be electrochemically active as proved by cyclic voltammetry and electrochemical impedance spectroscopy. In the optimized conditions, the Differential pulse voltammetry technique shows the responsive behavior to the nitrofurantoin antibiotics even at a very high linear range of concentrations (0.1-1000 ng/mL) with R2 =0.993. The limit of detection of 0.07 ng/mL and the limit of quantitation of 0.2 ng/mL was attained in a short response time on this electrochemical platform. The selectivity studies with other antibiotics were also studied. As a highlight of this research work, the Zr MOF/PTh-based detection platform for nitrofurantoin antibiotics with improved performance due to graphite foil with high current -collector electrode. In addition to this, improved sensitivity has been achieved over many of the previously reported electrochemical sensors.

ACKNOWLEDGMENTS

The presenting author is thankful to DBT India for the funding. SS and AD is thankful to Government of India, DBT-DFG integrated Project (IC-12025(11)/3/2020-ICD-DBT) in CSIR-CSIO,Chandigarh. PG is thankful to Herz Fellowship at University of Konstanz launched by Alexander-von-Humboldt-Stiftung. DB is thankful to CSIR-India for SRF.

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Unveiling the Mechanism of 2d, Quasi-2d and 3d Halide Perovskite Thin Films Formation

Thierry Pauporté*, Daming Zheng
CNRS – Institut de Recherche de Chimie-Paris (France)

* thierry.pauporte@chimieparistech.psl.eu

Abstract ID #NEE-524

Metal halide perovskites (PVK) have emerged as one of the most promising family of materials for applications in various fields such as lasers, light emitting diodes, photodetectors, scintillation and photovoltaic solar cells.[1,2] This material family exhibits excellent optoelectronic properties, tunable bandgap, long charge carrier lifetime, low-cost and low-temperature solution processibility. PVK thin films can be printed on flexible substrates for lightweight devices. In PVK-based optoelectronic devices, especially in photovoltaic solar cells, the growth control and the optimization of the film material quality are key to reach high efficiency. [1,2] We have investigated the solvent and perovskite elements' location and evolution upon the film processing steps. For this study, we focused on the technique employed for the preparation of efficient solar cells: spin coating, anti-solvent dripping and annealing.[3] 2D, Quasi-2D and 3D perovskite films formations with various compositions have been investigated. We show that the solvent always accumulates in the upper part of the initial layer, while lead is concentrated in its lower part. Moreover, solvent is eliminated in two steps upon annealing. Importantly, we show the key role of solvent elimination. We propose a taxonomy which distinguishes three types for the growth direction of perovskite crystals: downward, upward and lateral.[4] Among them, high efficiency and high stability always occur in samples with a lateral growth that can be governed with additives.

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Improvement of Perovskite Nanocrystals Stability by Incorporation into Polymer Cross-Linked Systems

Tamara Skrypnyk[1*], Maryna Bodnarchuk[2, 3], Maksym Kovalenko[2, 3], Iryna Bespalova[1], Luciano Boesel[2]
[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *EMPA, Swiss Federal Laboratories for Materials Science and Technology (Switzerland)*
[3] *Institute of Inorganic Chemistry, ETH Zürich (Switzerland)*

* tamara.skrypnyk@empa.ch

Abstract ID #NEE-556

In recent years, the interest of many scientists in all-inorganic metal halide perovskite nanocrystals with can be obtained both in form of colloidal solutions and powders has increased rapidly due to their attractive properties and promising applications [1,2]. A feature of all-inorganic halide perovskites is that a width of a bang gap can be tuned by varying proportions between precursors, which gives a wide range of luminescence maxima from the blue to red regions [3]. Due to the quantum-dimensional effect perovskites have a quick nanosecond luminescence of free excitons with a high quantum yield.

However, these materials have the disadvantage of chemical instability - they are sensitive to moisture, temperature, and light, which limits all their technological applications [4]. To overcome this issue, these nanocrystals can be combined with other classes of materials such as different types of polymers, silica, and others [5].

In this research, we investigated composites of perovskite nanocrystals CsPbX3 (X = Br, Cl) with polymer networks to enhance the optical properties and stability of nanocrystals for further practical applications (e.g. energy harvesting, detection, and imaging instruments). Parameters investigated include the methods of synthesis of perovskite nanocrystals (hot-injection method and LARP technique), type of ligand, type and chemical composition of a network (hydrophobic and amphiphilic), and network nanostructure. Our results demonstrate different options for the improving the stability and luminescence of nanocrystal composites with polymer cross-linked systems on these materials under a various external conditions.

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Nitrogen-Doped Porous Carbon Derived From Hemp Hurd as Electrode for Aqueous Supercapacitors

Volodymyra Boychuk[1], Bogdan Rachiy[1], Ruslan Zapukhlyak[1], Volodymyr Kotsyubynsky[1] *, Mykola Hodlevskyi[1], Rashad G. Abaszade[2]

[1] *Vasyl Stefanyk Precarpathian National University (Ukraine)*
[2] *Azerbaijan National Academy of Sciences (Azerbaijan)*

* kotsuybynsky@gmail.com

Abstract ID #NEE-558

Activated carbons were obtained from hemp hurd using carbonization at 800°C and chemical activation with KOH (HC sample). The carbonization process of raw material includes (thermal analysis data) the decomposition of hemicellulose (210-330oC), lignin depolymerization (350-500°C), and decomposition of cellulose (up to 600-700°C). The treatment with nitric acid at 70°C in N2 flow allows obtaining N-doped carbon where nitrogen atoms are included in N–CH3 surface functionalities (FTIR data) (HC-N sample). The additional thermal treatment of nitrogen-doped carbon was performed at 400°C (HC-NO sample). The presence of both micro- and mesopores was observed for all obtained samples with the mesopores content increasing after nitrogen doping and annealing with the BET specific surfa¬ce area values of 855, 1108, and 1280 m2/g for HC, HC-N, and HC-NO samples. The pore sizes (calculation using NLDFT, slit-like pores appro¬ximation) for the HC sample are mostly <5 nm with the micropores and mesopores at equal volumes. Additional acid treatment of HC and next annealing affect both the concentration and distribution of micropores and the formation of new mesopores with sizes up to 20 nm [1]. The analysis of Raman spectra allows calculating the average sizes of graphite crystallites as a structural element of the turbostratically ordered porous carbon. The average lateral size (in the direction parallel to (002) crystallography plane) of graphite clusters are about 6.6, 6.0 and 5.9 nm for HC, HC-N and HC-NO samp¬les, respectively. The electrochemical performance using galvano¬static charge/discharge cycling was tested for symmetric configuration using 6 M KOH aqueous electrolyte. The charge-discharge curves (CDCs) of HC supercapacitor are close to triangular (with inner resistance causing a voltage drop up to 0.18 V) that indicates a double electric layer mechanism of charge storage. In contrast, both branches of CDCs for HC-N-based supercapacitor is distorted due to the presence of a Faradaic reaction. The IR drop decreasing (up to 0.10 V) corresponds to conductivity increasing and charge transport optimization. The increase of IR drop (up to 0.15 V) for HC-NO-based supercapacitor is observed. The specific capacitance values of 110, 150, and 115 F/g were observed for HC, HC-N, and HC-NO-based supercapacitors after 100 cycles at Coulomb efficiencies of 99.0, 97.8, and 98.8 %, respectively. The best performance of nitrogen-doped carbon samples is caused by pseudo¬capacitance and electron-donor properties of nitrogen surface functionalities [2]. The removal of nitro¬gen-containing groups after annealing leads to capacitance decreasing at the respectively highest specific surface area.

ACKNOWLEDGMENTS

This work was funded by the National Research Foundation of Ukraine (2020.02/0043).

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Structure and Properties of Visible-Light Active Binary TiO_2 & Au Nanocomposites

Olena Mykolaivna Lavrynenko[1] *, Maksym Zahornyi Mykitovich[2], Olesja Pavlenko Yuriivna [2], Erwan Paineau[3]

[1] *I.M. Frantsevich Institute for Problems of Material Science of National Academy of Science of Ukraine (Ukraine)*

[2] *I.M. Francevich Institute for Problems of Materials Science NAS of Ukraine (Ukraine)*

[3] *Laboratoire de Physigue des Solides Universite Paris-Saclay (France)*

* alena.lavrynenko@gmail.com

Abstract ID #NEE- 562

Today, the creation of new and improvement of existing photocatalytic nanomaterials is one of the most urgent tasks of modern materials science. In particular, titanium dioxide-based photocatalysts have been successfully used to degrade organic dyes, but require exposure to visible light, which is explained by the semiconductor's wide band gap of 3.2 eV. One way to extend the action of titanium oxide catalysts to the visible light region is to modify them with substances of a different nature, such as noble metals. We have carried out a chemical synthesis of binary nanocomposites based on TiO2 modified with gold in the range of dopant concentration from 0.5 to 3.5 wt%. Titanium tetraisopropoxide was chosen as a titanium oxide precursor compound, and aurum aquaforms were obtained from a solution of gold hydrofluoric acid. The composition, structure, and morphology of nanocomposite particles were determined and their photocatalytic activity was tested under visible light for the destruction of malachite green (MG). The initial dye solution contained 20 mg/dm3 of MG at a pH of 6.8. By X-ray phase analysis, it was found that calcination of all lyophilized titanium-aurum-containing precipitates at T 600 C leads to the formation of anatase particles, and an increase in the treatment temperature to 1000 C promotes only a partial polymorphic transformation of anatase into rutile. The calculation of the crystal lattice parameters of anatase suggests that gold forms clusters on its surface. At the same time, it is possible that aurum cations may partially enter the anatase lattice, which requires further investigation. The size of anatase particles varies from 9.2 to 12.3 nm, and the size of rutile particles reaches 35 nm. Photocolorimetric measurements of the degree of destruction of the MG were performed according to the standard method after the system reached equilibrium for 30 minutes of stirring the suspension in the dark. A centrifuge with a capacity of 8 g was used to precipitate the nanoparticles in order to prevent their influence on the measurement results. The results proved that all samples of gold-modified anatase have a high efficiency of solution decolorization, which is 88-95% within 10-20 minutes. The best result was obtained for the sample with a 2 wt.% admixture content. The decolorization efficiency decreased to 45-53 % after heat treatment of the samples at T 1000 C. Further studies of particles of nanocomposites based on titanium dioxide modified with gold will be aimed at determining the effect of pH and dye concentration on the efficiency of its destruction. Attention will also be paid to the possibility of regeneration of the composite particles and evaluation of their stability under the influence of the dye. It is also planned to make a comparative characterization of the effectiveness of particles of coated composites under the influence of UV irradiation and visible light regarding the destruction of MG solution

Structure and Properties of Visible-Light Active Binary TiO_2 & Au Nanocomposites

Olena Mykolaivna Lavrynenko[1] *, Maksym Zahornyi Mykitovich[2], Olesja Pavlenko Yuriivna [2], Erwan Paineau[3]

[1] *I.M. Frantsevich Institute for Problems of Material Science of National Academy of Science of Ukraine (Ukraine)*

[2] *I.M. Francevich Institute for Problems of Materials Science NAS of Ukraine (Ukraine)*

[3] *Laboratoire de Physigue des Solides Universite Paris-Saclay (France)*

* alena.lavrynenko@gmail.com

Abstract ID #NEE-563

Today, the creation of new and improvement of existing photocatalytic nanomaterials is one of the most urgent tasks of modern materials science. In particular, titanium dioxide-based photocatalysts have been successfully used to degrade organic dyes, but require exposure to visible light, which is explained by the semiconductor's wide band gap of 3.2 eV. One way to extend the action of titanium oxide catalysts to the visible light region is to modify them with substances of a different nature, such as noble metals. We have carried out a chemical synthesis of binary nanocomposites based on TiO2 modified with gold in the range of dopant concentration from 0.5 to 3.5 wt%. Titanium tetraisopropoxide was chosen as a titanium oxide precursor compound, and aurum aquaforms were obtained from a solution of gold hydrofluoric acid. The composition, structure, and morphology of nanocomposite particles were determined and their photocatalytic activity was tested under visible light for the destruction of malachite green (MG). The initial dye solution contained 20 mg/dm3 of MG at a pH of 6.8. By X-ray phase analysis, it was found that calcination of all lyophilized titanium-aurum-containing precipitates at T 600 C leads to the formation of anatase particles, and an increase in the treatment temperature to 1000 C promotes only a partial polymorphic transformation of anatase into rutile. The calculation of the crystal lattice parameters of anatase suggests that gold forms clusters on its surface. At the same time, it is possible that aurum cations may partially enter the anatase lattice, which requires further investigation. The size of anatase particles varies from 9.2 to 12.3 nm, and the size of rutile particles reaches 35 nm. Photocolorimetric measurements of the degree of destruction of the MG were performed according to the standard method after the system reached equilibrium for 30 minutes of stirring the suspension in the dark. A centrifuge with a capacity of 8 g was used to precipitate the nanoparticles in order to prevent their influence on the measurement results. The results proved that all samples of gold-modified anatase have a high efficiency of solution decolorization, which is 88-95% within 10-20 minutes. The best result was obtained for the sample with a 2 wt.% admixture content. The decolorization efficiency decreased to 45-53 % after heat treatment of the samples at T 1000 C. Further studies of particles of nanocomposites based on titanium dioxide modified with gold will be aimed at determining the effect of pH and dye concentration on the efficiency of its destruction. Attention will also be paid to the possibility of regeneration of the composite particles and evaluation of their stability under the influence of the dye. It is also planned to make a comparative characterization of the effectiveness of particles of coated composites under the influence of UV irradiation and visible light regarding the destruction of MG solution

Effect of the Adsorbed on the Nanoparticles Surface Air Components on the Nanofluid Colloidal Stability: an Experimental Study

Volodymyr Borysov[1], Bohdan Kvasnytskyi[1, 1], Nikita Khliiev[2] *, Vitaly Zhelezny[1], Vladimir Gotsulskiy[2]
[1] *Odesa National University of Technology (Ukraine)*
[2] *Odesa I. I. Mechnykov National University (Ukraine)*

* khliyevn@gmail.com

Abstract ID #NEE-581

Nanofluids (NFs) can be considered promising working fluids and coolants for power systems. Nanoparticles (NPs) admixtures in liquids significantly affect their thermophysical properties. Thermophysical properties variation and colloidal stability of the NFs are determined by the concentration, size and shape of the NPs and by the influencing the NPs on the base liquid internal structure. Moreover, the NPs in the base liquid inhere in the presence of the surface layer of various air components that was sorbed during NPs' storage. For today, the effect of the sorbed layer on the NPs' surface on the colloidal stability of NFs has not been examined adequately. Here we demonstrate that preliminary NPs treatment to remove sorbed air components before NFs preparation contributes to obtaining the NFs with enhanced colloidal stability. Experimental studies of the desorption process regarding five different types of NPs that were stored under loose-fitting cover at the ambient conditions resulted that the adsorption layer consists mainly of water. For γ-Al2O3 NPs (specific surface area 120 m2/g) mass fraction of the adsorbed water was 2.2 %. Correspondingly, the following results have been obtained: Al2O3 NPs (8.7 m2/g) - 0.66 %; TiO2 (anatase, 49.5 m2/g) - 0.77 %; TiO2 (rutile, 41 m2/g) - 0.20 %; CuO (65.4 m2/g) - 0.19 %. A technique for the NFs preparation has been developed. This technique involved preliminary NPs treatment by vacuuming together with heating up to 200 °C, followed NPs milling with liquid and subsequent sonication. The measured hydrodynamic size (DLS) of the NPs aggregates in the NF obtained by the technique mentioned above was smaller than for similar NF prepared without NPs pre-treatment. The obtained results will contribute to improving the technique of preparation of the colloidal stable working fluids and coolants for power systems with high efficiency.

Experimental Study for the Enthalpy of the Diffuse Phase Transitions of Fullerene C60 Solutions in Industrial Paraffin Wax

Vitaly Zhelezny[1], Yana Hlek[1], Dmytro Ivchenko[1], Olga Khliyeva[2] *
[1] *Odesa National University of Technology (Ukraine)*
[2] *National University "Odessa Maritime Academy" (Ukraine)*

* khliyev@ukr.net

Abstract ID #NEE-583

Thermal energy storage (TES) units are an integral part of renewable and heat recovery power systems. Utilizing the phase change materials (PCMs) in TES units is considered to be a promising way to improve the efficiency of the power systems. The thermophysical properties of the PCM significantly affect the overall efficiency of the TES units. Nanotechnologies application is a long-term direction for improving the thermophysical properties of the PCMs for TES. Here we show that doping the industrial paraffin wax (PW) with fullerene C60 affects the value of enthalpy of the diffuse phase transition of composite PCM PW/C60 vs. pure PW. The conducted experiments indicated that the effect of C60 on the caloric properties of PW during heating and cooling is different. The presence of 0.000120 g·g-1 and 0.000746 g·g-1 of C60 in the industrial PW led to an increase in the crystallization enthalpy of composite PCM up to (19…25) % and up to (31…42) %, respectively. In contrast, a decrease in the melting enthalpy was recorded in the same temperature ranges. The obtained effects can be explained by the occurrence of the diffused phase transitions in a wide temperature range and by the influence of C60 fullerene admixtures on the internal structure of the PW in the liquid and solid phases. The obtained effects of C60 on the PW enthalpy of phase transitions indicate the expediency of further examination of the thermophysical properties of the various organic PCMs containing C60. The industrial implementation of the new generation of PCMs containing C60 will contribute to improving the efficiency of the TES units.

ACKNOWLEDGMENTS

The authors are grateful to the National Research Foundation of Ukraine, project № 2020.02/0125, for the financial support of this study

Intrinsic Properties of N-Doped Reduced Graphene Oxide on Manganese-Based (Oxides and Phosphates) Nanoparticles as Electrode Materials for Supercapacitors

Katlego Makgopa*
Tshwane University of Technology (South Africa)

* MakgopaK@tut.ac.za

Abstract ID #NEE- 596

Renewable energy (RE) has emerged as a key solution to mitigating the negative effects brought by the use of fossil fuels. It also provides hope for meeting the rising global energy demand. However, the effectiveness of RE relies on the incorporation of electrochemical energy storage (EES) systems for the sustainable application [1], [2]. Supercapacitors, as one of the promising EES systems, have stood out amongst energy storage devices due to their ability to deliver robust power outputs while being able to still retain their stability and efficiency after long charge-discharge cycles. The performance of supercapacitors is dependent on the physicochemical properties of the electrode materials. Hence, a robust design and optimization of the properties of electrode materials are necessary to enhance the energy storage performance of supercapacitors [3]. Combining the high stability, high surface area, and excellent electronic conductivity of the heteroatom-doped carbon material with the excellent ionic conductivity of the manganese-based oxides and phosphate results in a synergy of the properties useful for enhancing the energy storage performance of SC devices [3, 4].

Hence this work focuses on the integration of the non-Faradaic charge storage mechanism of N-rGO with the Faradaic charge storage of either Mn3O4 or NH4MnPO4·H2O as a vital approach toward the construction of supercapacitors with improved energy and power outputs. The prepared nanocomposites displayed excellent supercapacitive performance with high energy densities.

ACKNOWLEDGMENTS

KM is grateful for the financial support from the National Research Foundation, South Africa, under the Thuthuka programme (UID nos. 117984 and 118113) and the Competitive Support for Unrated Researchers (UID no. 138085).

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Pyroresistive Properties of Segregated Composites Based on Pvc Containing Carbon Fillers

Oleksii Maruzhenko[1] *, Yevgen Mamunya[2], Maksym Iurzhenko[1], Roman Kolisnyk[1], Olha Masiuchok[1], Yevheniia Buinova[1], Marcin Godzierz[3], Sébastien Pruvost[4]

[1] *E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine (Ukraine)*
[2] *Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine (Ukraine)*
[3] *Center of Polymer and Carbon Materials, Polish Academy of Sciences (Poland)*
[4] *Université de Lyon, CNRS, Université Claude Bernard Lyon 1, INSA Lyon, Université Jean Monnet, UMR 5223, Ingénierie des Matériaux Polymères, F-69621 Villeurbanne Cédex, France (France)*

* a.v.maruzhenko@gmail.com

Abstract ID #NEE- 617

Polymer composites with pyroresistive properties (that generate heat when an electric current flows through them) have recently attracted attention due to the possibility of their use in various industries. In the production of such composites, semi-crystalline polymers are traditionally used, that have a large PTC effect, due to which the materials receive self-regulating properties. The aim of this study was to evaluate the pyroresistive properties of amorphous composites on the example of polyvinyl chloride containing carbon fillers and to check the presence of the PTC effect in such a system.

In this work, composites based on polyvinyl chloride (PVC) filled with various carbon fillers: carbon black (CB), carbon fibers (CF) and their mixture (CB/CF) were studied. The composites were formed in such a way that the conductive phase of the carbon filler formed an ordered segregated structure in the form of a network. This type of spatial distribution of the filler in the polymer matrix suggests a high level of conductivity at a low filler concentration due to its high local concentration of filler particles in the walls of the network.

The electrical-thermal characteristics of PVC-CB, PVC-CF and PVC-CB/CF composites were studied. The kinetic dependences of the temperature of the composites T=f(t) at various applied voltage U to the samples show its increase in time t and reaching the equilibrium value Te, which depends on the applied voltage according to a quadratic law, Te=T0+a U2. At the same time, the equilibrium temperature increased linearly with the level of electrical power P supplied to the sample, Te=T0+b P. In composites, the PTC effect appears, which consists in slowing down and stopping the growth of Te or decreasing its value with increasing applied voltage U above a certain U value.

The amount of heat gained by the sample through electrical power is equal to the amount of heat lost through radiation and convection from the surface of the sample. Accordingly, the parameter b, at the state of temperature equilibrium, can be given as b=(Te-T0)/P. The higher the value of b, the higher the efficiency of converting electrical power into heat. The b value is equal to 50 oC/W for the PVC-CB composite, while for the PVC-CF and PVC-CB/CF composites the parameter b is 37 and 38.5 oC/W. This indicates a higher efficiency of carbon black, since it is a nanofiller with a high specific surface area, which facilitates the transfer of thermal energy from the filler to the polymer matrix.

Thus, electrically conductive composites based on amorphous PVC thermoplastic have pyroresistive properties and exhibit the PTC effect, which makes them suitable for creating materials for applications in various fields of technology, for example, for heating water in conductive pipes, for anti-icing coatings, for heaters in medical equipment, as a heating element at welding PVC pipes, and etc.

Reduced Porous Graphene Oxide Network as High-Performance Supercapacitor Electrodes: Effect of Reduction Temperature

Vivek Kumar*, Karthick Raja K, T Anusuya
Indian Institute of Information Technology Design & Manufacturing Kancheepuram, Chennai-600127, India (India)

* vivek@iiitdm.ac.in

Abstract ID #NEE-628

Graphene oxide (GO) is a highly desirable candidate for supercapacitors [1]. Controlling physical and chemical properties by controlling the reduction temperature at ambient conditions is one of the simple and cost-effective routes to improve the performance of the supercapacitor electrode [2]. Reduction at ambient conditions causes de-oxygenation and restoration of sp2 carbon which adjusts the material's electrical properties and electrochemical performance. Here, the graphene oxide (GO) was synthesized and reduced at 200 oC, 300 oC, and 400 oC to obtain porous reduced GO (Pr-GO). FTIR spectroscopy was used to investigate the elimination of the oxygen functional group. Structural reconstruction was studied using Raman spectroscopy. The electrochemical response of the material was studied using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) in a three-electrode setup. The maximum specific capacitance of 243 F/g was obtained for 400 oC Pr-GO in an aqueous electrolyte. The Pr-GO based supercapacitor device exhibits noticeably high charge-discharge cyclic stability. This work demonstrated that GO reduced at ambient conditions is a convenient way to increase the production of electrode material on a commercial scale.

ACKNOWLEDGMENTS

Author (KRK) acknowledges the financial support from Ministry of Education, India. Authors acknowledge the financial support from IIITDM Kancheepuram.

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Hydrophobic Silica Aerogel-Like Nanomaterials for Potential Environmental and Health-Care Related Applications

Selay Sert Çok[1] *, Fatoş Koç[1], Zoltán Dudás[2], Nilay Gizli[1]
[1] *Ege University (Turkey)*
[2] *Centre for Energy Reseach (Hungary)*

* selay.sert@ege.edu.tr

Abstract ID #NEE- 629

Silica-based aerogels are sol-gel-derived nanoporous materials with many outstanding properties, such as high specific surface area, low density, and high porosity. Regarding their tunable surface chemistry, their hygroscopic properties can easily be adapted for many target applications. Hydrophobic silica aerogels have been proven to be a promising material in various applications, such as the absorption of organic liquids/oils, thermal insulation, and biotechnological applications. For example, superhydrophobic silica aerogels can possess self-cleaning ability due to the lotus effect, or they can reduce bacterial adhesion by having an easy removal capability of the bacterial cells before a thick biofilm is formed on the surface [1]. Developing porous materials that may have a bacteria-repelling character based on hydrophobicity is a recent strategy reported only by a few studies so far [2,3]. In fact, considering all the unique aspects like tailorable morphology and hydrophobicity, the development of such multi-purpose materials to be utilized in different fields is of great importance, and therefore, they are needed to be explored more. This study is devoted to synthesizing methyl-functionalized silica aerogel-like nanomaterials for potential environmental and biomedical applications. The materials were prepared via a two-step sol-gel method by choosing a hydrophobic organofunctional silane methyltrimethoxysilane (MTMS) as silica precursor with traditional tetra alkoxysilane tetraethylorthosilicate (TEOS) under ambient conditions with a similar approach reported in Ref.[4]. The samples were silylated with trimethylchlorosilane (TMCS) after gelation. The degree of methyl functionalization was investigated by varying the amount of MTMS added to sol mixture. After evaporative drying, the surface chemistry and the degree of methyl attachment were qualitatively determined via FTIR analysis. The sample exhibiting a lightweight monolithic structure with low density (0.09 g/cm3), high porosity (95.2 %), and superior hydrophobicity (θ>140°) was then subjected to batch oil sorption experiment to evaluate its performance as an adsorbent for environmental remediation applications. The material exhibited a high oil uptake capacity (12.3 g/g) and endurable adsorptive performance (up to 6 cycles). It also showed an impressive self-cleaning property. As a last step, the bacteria-repelling property of the same samples was tested via dip-inoculation in bacterial suspensions containing either Gram-negative Escherichia coli or Gram-positive Staphylococcus aureus. Bacterial attachment on the sample surfaces was observed via SEM analysis, and results have shown that, compared to its hydrophilic counterparts, the hydrophobic sample displayed a significant bacterial anti-adhesion characteristic. All these features could make these materials exceptional candidates to participate in many future environmental and biomedical-related applications efficiently.

ACKNOWLEDGMENTS

This abstract is based upon work from COST Action AERoGELS CA18125 (Advanced Engineering and Research of aeroGels for Environment and Life Sciences), supported by COST (European Cooperation in Science and Technology.

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Catalytic Activity Assessment of APS Glass Sprayed Sno2/Zro2 Coatings In the Light Activated Degradation Of Eosin Y and Toluidine Blue

Alicja Duda[1, 2] *, Bartosz Kopyciński[3, 2], Monika Czerny[1], Krzysztof Pęcak[1, 2], Marcin Lis[1], Adriana Wrona[1]

[1] *Łukasiewicz Research Network - Institute of Non-Ferreous Metals (Poland)*
[2] *Doctoral School, Silesian University of Technology (Poland)*
[3] *Łukasiewicz Research Network - Institute for Engineering of Polymer Materials and Dyes (Poland)*

* alicja.duda@imn.lukasiewicz.gov.pl

Abstract ID #NEE- 630

The industrial-origin organic wastes are considered to be one of the main reasons for soil and water pollution [1]. The search for efficient and easy-accessible methods for the removal of organic pollutants is still a topic of many scientific discussions. Among them, in around past 15 years, many reports widely discuss the application of nanomaterials in wastewater treatment [2].

The presented work is focused on the analysis of the catalytic activity of thermally sprayed SnO2, ZrO2 and SnO2/ZrO2 coatings on the example of Eosin Y and Toluidine Blue light activated degradation. Nanopowders of SnO2 and ZrO2 in different mass ratios were applied as raw materials for the fabrication of coatings on glass in the process of atmospheric plasma spraying. As part of the research, powders properties such as specific surface area, actual density or flowability were characterized. Phase and chemical composition analysis of both powders and coatings was performed via electron probe X-ray microanalysis and X-ray powder diffraction methods. The morphology and the geometric structure of the surface of the SnO2/ZrO2 coatings were investigated. Catalytic degradation of Eosin Y and Toluidine Blue with the use of powder raw materials and obtained coatings as photocatalysts were carried out in aqueous dyes solutions in a photoreactor operating in the visible light range. Moreover, color measurements of catalysts before and after the photodegradation processes were carried out using a sphere spectrophotometer in the CIELab color space. The profilometry measurements with roughness parameters stated at 75÷87 and 95÷103 µm for maximum peak-to-valley height Rz and maximum roughness depth Rmax indicate the disordered directivity of the surface of the coatings. X-ray powder diffraction confirmed chemical composition free of impurities, and the presence of only SnO2 and ZrO2 phases, both in powders and coatings. It was shown that all of the tested SnO2/ZrO2 coatings exhibit the ability to the degradation of Eosin Y and Toluidine Blue after exposure to light. The most effective in the removal of both dyes were coatings containing 100% and 85% SnO2.

The obtained results confirm the possibility of using ceramic glass coatings in the processes of degradation of toxic organic substances from the aqueous environments. Furthermore, taking into account the attainability of raw materials and the inexpensive manufacturing process, such coatings can be an attractive solution for environmental protection in many branches of science and industry [3].

ACKNOWLEDGMENTS

This work was financially supported by subvention of Polish Ministry of Education and Science for Łukasiewicz Research Network – Institute of Non-Ferreous Metals for a year 2022.

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The Effect Of Hydrogen and its Mixtures With Natural Gas on Structure of Technical Polyethylene

Maksym Kovalchuk[1] *, Maksym Iurzhenko[1], Valeriy Demchenko[2], Valeriy Verbovsky[3], Hennadiy Zhuk[3], Leonid Unigovskyi[4], Igor Gotsyk[5], Marcin Godzierz[6]

[1.] *E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine (Ukraine)*
[2.] *Institute of Macromolecular Chemistry, NAS of Ukraine (Ukraine)*
[3.] *Institute of Gas of the National Academy of Sciences of Ukraine (Ukraine)*
[4.] *Naftogazbudinformatyka, ltd. (Ukraine)*
[5.] *Ltd "Regional gas company" (Ukraine)*
[6.] *Center of Polymer and Carbon Materials, Polish Academy of Sciences (Poland)*

* KovalchukMAwork@gmail.com

Abstract ID #NEE- 634

The study of the long-term effect of hydrogen and its mixtures with natural gas on the structure of technical polyethylene, which is used for the production of pipes, allows determining the possibility of their transportation through polyethylene pipelines. In the present work, polyethylene samples were exposed to hydrogen mixtures for 6 months. In order to establish the dependency between the degree of influence and concentration of hydrogen, mixtures of 10% H2/90% CH4 and 20% H2/80% CH4 were used. Before starting the experiment, in order to indicate possible changes in the structural characteristics of polyethylene, the following studies were also carried out on input samples that were not exposed to hydrogen mixtures.

The structural studies showed the influence of both gas mixtures on the structure of polyethylene, in particular the crystalline phase. A decrease in the size of crystallites and their orderliness under the influence of gas mixtures in the volume of samples was revealed. At the same time, the appearance of crystallites of a new shape was found on the surface of the samples. The effect of gas mixtures on polyethylene has physical nature since no changes in the chemical structure of the polyethylene were detected.

It is assumed that the change in the structure of the crystalline phase is caused by the competing action of hydrogen and methane molecules, while methane can act as a polyethylene solvent, which is accompanied by a slight swelling of polyethylene and minor structural changes of a physical nature. In this case, hydrogen molecules contribute to the formation of smaller crystallites of a new shape.

ACKNOWLEDGMENTS

The present research is conducted in close cooperation and under funding of Ltd "Regional gas company" and Ltd "Naftogazbudinformatyka".

Zinc Ferrite Nanoparticles as Electrode Material for Photo-Supercapacitor

Piyali Chatterjee*, Kousik Pradhan, Shobha Shukla, Sumit Saxena
Indian Institute of Technology Bombay (India)

* piyali93physics@gmail.com

Abstract ID #NEE- 637

In the face of global energy crisis due to limited fossil fuels along with rising pollution, materials science research is focussed on renewable energy utilisation in line with United Nations' Sustainable Development Goals of affordable and clean energy to be met by 2030. Sun is an abundant energy source available on earth but it is discontinuous in nature. This has made storage mechanisms like batteries and supercapacitors to be essential along with harvesting technologies like solar cells. Recently, to avoid losses due to external connection, more compact solar energy conversion and storage systems [1] like integrated photoelectrochemical batteries and photo-assisted supercapacitors (PSC) have come up for efficient solar energy storage. This work deals with development of supercapacitors with low band gap electrode material to enable photo-assisted charging. [2] In this regard, a known pseudocapacitive bimetallic oxide, zinc ferrite (ZnFe2O4) powder has been synthesized by facile chemical precipitation. [3] The structural and morphological characterisation by X-ray diffraction and scanning electron microscopy revealed formation of nano-crystalline spinel ferrite particles. The electrochemical properties of the samples as investigated by Cyclic voltammetry, Galvanostatic charge discharge (GCD) and electrochemical impedance spectroscopy (EIS) in three electrode configuration revealed good areal specific capacitance and cycling stability of the material as negative electrode material in alkaline electrolyte (KOH). Asymmetric and symmetric photo-supercapacitor devices have also been fabricated with optimised ZnFe2O4 as active material drop-casted on transparent FTO glass substrate for the first time with PVA-KOH gel electrolyte cum separator and reduced graphene oxide based positive electrode. Photo-assisted enhancement of specific capacitance and cycling stability has been demonstrated. Therefore we propose this low cost stable oxide of earth abundant metals as a viable material for practical application in the development of photo-supercapacitors.

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Novel Strategies to Improve Nanostructured TiO_2 Properties for the Photocatalytic and Photoelectrocatalytic H_2 Generation

Ewa Wierzbicka*
Department of Functional Materials and Hydrogen Technology, Faculty of Advanced Technologies and Chemistry, Military University of Technology, 2 Kaliskiego Street, 00908 Warsaw, Poland (Poland)

* ewa.wierzbicka@wat.edu.pl

Abstract ID #NEE-654

"Green Deal" is a plan of the European Commission to reach climate neutrality by 2050. This forces fast switching from classic fossil fuels to new energy carriers such as hydrogen, which is so far the most promising candidate for their substitution. It is an energy carrier, which in ideal conditions of production and usage shows a zero-carbon footprint (combustion with oxygen produces pure water). Therefore, searching for novel technologies that can be used for renewable hydrogen production is very timely and highly relevant.

One strategy of sustainable hydrogen generation is based on photosensitive materials that can split water into hydrogen and oxygen using solar radiation. Since 1972, when Fujishima and Honda discovered the phenomenon of water photolysis from TiO2, it has become the benchmark semiconductor material tested for photocatalysis (PC) and photoelectrocatalysis (PEC). After these years, the PC/PEC hydrogen evolution from water are still not efficient enough to meet the economic criteria of commercialization, therefore further modifications are necessary to improve the material performance.

TiO2 can form various nanostructures such as nanopowders, and anodic nanotubes/nanoporous arrays, with many times higher surface area in comparison to bulk materials. Nanostructurization of the TiO2-based material itself strongly increases PC/PEC performances. Moreover, such materials show great potential for further modifications. On the one hand, the most efficient and frequently used approach to TiO2 modification is coupling it with noble metal cocatalysts such as Pt, Ag, Au, or their alloys [1,2]. This modification brings much higher PEC and PC process efficiencies assigned to several effects, such as Schottky barrier formation, co-catalytic properties into hydrogen absorption, or surface plasmon resonance. The processes that might take place at the metal-semiconductor interface are complex depending on the type of metal used in heterojunction. On the other hand, noble-metal-free modification strategies such as sensitization with other semiconductors [3], or so-called material self-doping, are becoming increasingly popular [4,5]. Here will be shown, how adequately designed modification of nanostructured titania can improve PC/PEC water-splitting performance by creating suitable electronic pathways to enhance spatial separation of photogenerated charge carriers.

ACKNOWLEDGMENTS

The research was financially supported by the Polish National Agency For Academic Exchange, Polish Returns Programme (Project No. BPN/PPO/2021/1/00002), and the National Science Centre, Poland (Project No. 2022/01/1/ST5/00019).

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Piezoelectric Nanogenerator Based On Flexible Polylactide/ Bismuth Ferrite 0-3 Type Polymer Composites

Olha Masiuchok[1*], Marcin Godzierz[2], Sébastien Pruvost[3], Aurélien Roggero[3], Urszula Szeluga[4], Maksym Iurzhenko[1]

[1.] *E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine (Ukraine)*
[2.] *Center of Polymer and Carbon Materials, Polish Academy of Sciences (Poland)*
[3.] *Université de Lyon, CNRS, Université Claude Bernard Lyon 1, INSA Lyon, Université Jean Monnet, UMR 5223, Ingénierie des Matériaux Polymères, F-69621 Villeurbanne Cédex, France (France)*
[4.] *Centre of Polymer and Carbon Materials, Polish Academy of Sciences (Poland)*

* omasiuchok@gmail.com

Abstract ID #NEE- 658

Recently, one can observe significant demand for energy harvesting technologies as a possible alternative to provide a continuous power supply for low-power devices in different applications. It causes to growing up the interest in research on piezoelectric nanogenerators (PENG) for the conversion of mechanical stress into electrical energy [1, 2]. The design and fabrication of such devices is a huge challenge considering the cost of the materials used in their construction [3, 4]. The most effective way to decrease the amount of piezoelectric phase is fabrication of polymer composites, where the active (piezoelectric) phase is dispersed in a polymer matrix [5].

The aim of this work was focused on the study of the impact of BiFeO3 (BFO) nanoparticles on piezoelectric performance of 0-3 polymer composites. For it two types of BFO particles – commercially available and fabricated by reverse co-precipitation method were used. Subsequently, the dispersion of particles in solvent was prepared using ultrasounds, what allows to destroy agglomerates created during sintering and obtain particles with size of approx. 200 nm.

The effect of BFO nanoparticles synthesis and theirs weight amount (1-20%) on the filler dispersion (SEM), structure (XRD), dielectric properties and piezoelectric response of polylactide/ bismuth ferrite thin films was investigated. The results of piezoelectric measurements allow to conclude that developed flexible nanocomposites based on PLA matrix and fabricated BFO nanoparticles showed good energy conversion efficiency. The highest values have been reached for the composites with 15 wt.% and 20 wt.% BFO. Average power output density of these composites for air steam pressure (11.54 bar) – 59.34 μW/cm2 and 57,27 μW/cm2, respectively. Detected values are close to the analogical results of composites with commercial BFO nanoparticles – 64,66 μW/cm2. Therefore, produced nanocomposites with fabricated BFO nanoparticles as a filler, besides many benefits like cost-effective, eco-friendly and simple manufacturing method, can be successfully used for gas pressure sensing and energy harvesting.

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An Experimental Investigation of the Caloric Properties for the Composite Phase-Change Material Paraffin Wax-Expanded Graphite

Vitaly Zhelezny[1], Dmytro Ivchenko[1], Yana Hlek[1] *, Olga Khliyeva[2]
[1.]*Odesa National University of Technology (Ukraine)*
[2.]*National University "Odessa Maritime Academy" (Ukraine)*

* yanaglek90@gmail.com

Abstract ID #NEE- 661

Efficient thermal energy storage (TES) is one of the pillars on the way to the reduction of greenhouse gas emissions. Energy density is a key parameter for the phase change materials (PCMs) for the TES systems. Therefore, the caloric properties of the new generation of composite PCMs require a deeper examination. Here we show that impregnation of the expanded graphite (EG) matrix with industrial paraffin wax (PW) contributes to an increase in the value of enthalpy of the diffuse phase transition for the composite PCM PW/EG in comparison with pure PW. For this purpose, the PW/EG samples were explored in terms of the effective heat capacity over a wide temperature range. The mass fraction of the EG in the PW varied in the range from 3.2 to 6.5 %. The effect of the EG on the PW caloric properties, measured during heating and cooling, was different. It was found that the formation of the adsorption structured layer from the PW molecules on the surface of the EG matrix during cooling requires additional energy. Therefore, it is a reason for the significant increase in the crystallization enthalpy of the PW/EG samples vs. theoretical value. On the contrary, the EG matrix suppresses thermal fluctuations that contribute to the destruction of metastable structures in the liquid PW. It may explain the decrease in the melting enthalpy of the PW/EG samples vs. the theoretical value. The increase in the EG mass fraction above the lower concentration of the PCM stability - 3.2% - does not lead to a significant variation in the value of phase transition enthalpy. The obtained effects indicate the expediency for further search of the optimal EG concentration in the various organic PCMs. The industrial implementation of the new generation of PCMs containing EG will contribute to improving the efficiency of the TES units.

ACKNOWLEDGMENTS

The authors are grateful to the National Research Foundation of Ukraine, project № 2020.02/0125, for financial support of this study.

Evaluation of Long-Term Disinfection Efficacy of Silver Nanoparticle Immobilised Chitosan Composite Coated Sand In Groundwater By Breakthrough Curves Analysis and Regeneration

Naga Jyothi MSV *, Amesh P, Ramaiah B.J, Maliyekkal S.M
Indian Institute of Technology Tirupati (India)

* ce21d502@iittp.ac.in

Abstract ID #NEE- 662

Provision of safe drinking water is one of the sustainable development goals of United Nations. The stress of unavailability of microbial-free potable water is severe in rural areas and urban slums arising health problems, mortality, and economic loss. Provision of centralised treatment system involves high capital cost which is an economic burden in the developing and underdeveloped countries [1]. Hence there is an immediate requirement of safe, low-cost, efficient, and decentralised household point-of-use disinfection system.

Direct use of conventional chlorine-based disinfectants produces toxic and cancerous disinfection byproducts like trihalomethanes and halo acetic acids in treated water. On contrary, silver nanoparticles are proven to be commendable in terms of broad spectrum of antimicrobial property, efficacy, and facile synthesis compared to other metal nanoparticles like copper and zinc. In sight of field application, these nanoparticles have to be coated/immobilised on a suitable substrate to prevent the nanotoxicity from treated water enabling controlled release of silver. Majority of the publications were not conversed about the long-term disinfection performance of such nanoparticles loaded substrates which is the need of the hour.

In the present work, a facile and scalable synthesis protocol is developed for silver nanoparticle immobilised chitosan composite coating on sand (AgNC-sand) for water disinfection. Column studies are performed in a fixed bed reactor of 2 cm diameter for analysing silver leaching and disinfection efficacy. The proposed synthesis protocol enabled controlled and persistent release of silver ions from the substrate in to the groundwater matrix within the permissible limit of drinking water. The leaching mechanism of silver ions from the silver nanoparticle embedded coated sand involves swelling of polymer and oxidative dissolution. Breakthrough curve behaviour is interpreted by modelling the data of varying flow rate (15, 25, and 50 mL/min), bed depth (3.5, 7, and 14 cm) and input Escherichia coli conditions (101, 103, and 105 CFU/mL) in groundwater matrix. It was observed that the leaching and disinfection efficacy of the system is reduced after sometime due to deposition of salts like calcium, silica, magnesium from water. AgNC-sand when packed in a cartridge (500 g), it treated nearly 2500 L of groundwater, serving a family of 5 with 4 L/d demand for 4 months. An intermittent hot water regeneration was performed to remove deposited salts which was confirmed by FESEM imaging. Preliminary studies are performed to enhance the regeneration of system by chemicals like sodium citrate, citric acid, and ethanol. It was elucidated that the citric acid regeneration is efficient when compared to other chemicals.

ACKNOWLEDGMENTS

The authors acknowledge the Department of Science and Technology (DST)-Water Technology Initiative (DST/TM/WTI/WIC/2K17/82) for funding the work.

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Effect of Gaas Substrate Orientations and Doping On The Electrical and Optical Properties of Ingap Solar Cell Structures

Saud Alotaibi[1], Mozart Correa Avila [2], Labed Madani[3], Abdulaziz Almalki[4], Soltan Alhassan[5], Maryam Al Huways[6], Yara Galvao Gobato[2], Hassanet Sodabanlu[7], Masakazu Sugiyama[7], Helder Vinicius Avanco Galeti[2] *, Noureddine Sengouga[3], Mohamed Henini[1]

[1] *University of Nottingham (United Kingdom)*
[2] *Federal University of São Carlos (Brazil)*
[3] *University of Biskra (Algeria)*
[4] *Taibah University-Yanbu (Saudi Arabia)*
[5] *Jouf University (Saudi Arabia)*
[6] *Princess Nourah bint Abdulrahman University (PNU) (Saudi Arabia)*
[7] *The University of Tokyo (Japan)*

* helder@ufscar.br

Abstract ID #NEE- 664

High-performance optoelectronic devices based on InGaP have been fabricated as a promising material choice for space and concentrated photovoltaic applications due its large direct band gap of 1.9 eV and superior radiation resistance. However, depending on the growth conditions and substrate orientation, CuPtB-type ordering can appear in lattice-matched InGaP-on-GaAs layers [1,2]. Furthermore, localization and delocalization of carriers may simultaneously exist due antiphase boundaries (APBs) at the boundary of ordered domains, which has been well shown to produce a pronounced impact on the electrical and optical properties of materials [3]. This work investigates the effect of the GaAs substrate orientation ((100) and (100) 20off towards (111B)) and doping on the electrically and optically active defects in p-(i/n)-n GaAs/In0.48Ga0.52P/GaAs solar cell heterostructures grown by metalorganic chemical vapor deposition (MOCVD). The sample's electrical properties were investigated using current density-voltage, capacitance-voltage and deep-level transient spectroscopy (DLTS) techniques, which revealed electron and hole traps attributed to the DX center and vacancy-related defects such as VIn or VGa, respectively. Photoluminescence spectroscopy (PL) as a function of temperature and laser power dependence has evidenced different emission bands which were associated with excitonic and free carriers transitions in InGaP disordered regions, besides spatially indirect transition in ordered domains transitions involving electrons at donors and photoexcited holes. Furthermore, the PL spectra were also affected by distinct degrees of atomic ordering between the samples, rising the ordering domains for tilted substrate orientation as compared with doped (100) orientation, with n-doping effect showing a reduced ordering as compared to undoped exact (100) sample.

ACKNOWLEDGMENTS

This work was supported by "Fundação de Amparo à Pesquisa do Estado de São Paulo (grant numbers 2019/23488-5 and 19/07442-5) and "Conselho Nacional de Desenvolvimento Científico e Tecnológico" (CNPq)

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Modified CdTe Layers

Tetiana Mazur[1] *, Myroslav Mazur[2]
[1] *Ivano Frankivsk National Technical University of Oil and Gas (Ukraine)*
[2] *Ivano-Frankivsk National Technical University of Oil and Gas (Ukraine)*

* tetiana.mazur@nung.edu.ua

Abstract ID #NEE- 666

The study of the possibilities of improving the properties of CdTe with a view to its application in solar energy requires finding technological solutions to improve the quality of the material and the structures based on it. To date, surface barrier diodes have been developed with an efficiency of about 13% achieved at a temperature of 300 K under AM2 sunlight conditions [1]. The main idea of this technology is the preliminary annealing of low-resistance n-CdTe substrates under certain conditions in air, which leads to the formation of a near-surface layer, which significantly improves the photoelectric characteristics of diode structures.

Studies have found that the resistivity of the formed layer is much higher than that of the original substrate. The depth of occurrence of electrically active donor levels, determined from the temperature dependences of conductivity, is 0.14 and 0.33 eV, although annealing leads only to a decrease in electrical conductivity without changing its type [2]. We also study the physical reasons for possible changes in the crystal and energy structure of the modified layer compared to the base crystals.

According to the λ-modulated spectral distribution of the short-circuit current of two diodes fabricated on the original and annealed n-CdTe crystals, the semitransparent gold contact, through which illumination is produced in the spectral range under study, is almost uniform. The features in the differential spectra of Sω' are due only to singularities in the energy structure of CdTe. The cross-section Sω' with the abscissa axis is 1.5 eV and is consistent with the band gap of Eg CdTe at 300 K, which remains unchanged and additionally confirms that the base substrates and the modified layer have the same lattice constant.

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Nanocomposite Polymer Fibers for Selective Removal of Cesium Radionuclides From High Salt Solutions

Yuliia Bondar[1] *, Svetlana Kuzenko[2], Kostyantyn Yaroshenko[2], Dmytro Charnyi[2]
[1] *Czech University of Life Sciences Prague, Kamýcká 129, 165 00, Prague – Suchdol, Czech Republic (Czech Republic)*
[2] *State Institution "The Institute of Environmental Geochemistry of National Academy of Sciences of Ukraine" (Ukraine)*

* juliavad@yahoo.com

Abstract ID #NEE- 673

^{137}Cs radionuclides are the main component of liquid radioactive waste (LRW) formed owing to the operation of nuclear facilities. Due to their long half-life (~ 30 years), and high chemical activity, and radioactivity as a gamma-ray emitter, cesium radionuclides pose a considerable threat to human health. Therefore, the treatment of liquid radioactive waste to a safe level is a crucial key to the sustainable development of nuclear energy.

Among the handling methods developed for the removal of ^{137}Cs from contaminated waters, selective adsorption is the simplest and most economical one. Transition metal ferrocyanide nanoparticles (FC NPs) are highly selective to cesium ions; however, they have not found wide practical applications as adsorbents due to low hydromechanical stability. In the last decade, a variety of techniques have been developed for the synthesis of composite adsorbents by incorporating the FC NPs into the appropriate solid supporting matrix to improve their hydromechanical strength and adsorption characteristics.

We fabricated nanocomposite adsorbent for cesium ions by direct formation of potassium copper ferrocyanide NPs on the polyacrylonitrile fibers. The scanning electron microscope data revealed the rounded FC NPs (40-60 nm), uniformly distributed within the fibers' volume. The synthesized composite fibers demonstrated rapid adsorption, high adsorption capacity, and good chemical stability over a wide pH range. The composite fibers have demonstrated a high cesium removal efficiency (89%) from a multi-component model solution with a high salt content (~70 g/l), which confirmed their high selectivity to cesium ions.

The synthesized composite fibers can be recommended for the decontamination of seawater and low-level LRW with high salt content. The great advantage of synthesized composite fibers is their simplicity of manufacture, low cost due to the use of inexpensive commercially available polyacrylonitrile fibers, fast adsorption, high adsorption capacity, and high selectivity to cesium ions.

Synthesis of Silcia Nanoparticles from Rice Husk and Their Applications In Soil Remediation

Anu Gupta*
Guru Jambheshwar University of Science & technology, Hisar, haryana, India (India)

* anu339@gmail.com

Abstract ID #NEE- 683

Agriculture waste is a big burden on the earth due to farming activities in developed and developing countries. It causes severe pollution problems when they are burnt openly . It is important to manage this waste in a proper manner. Several efforts have been made over past decades to combat the situation. One such effort is the integration of nanotechnology for utilizing waste and offers two-fold benefit. First is the utilization of waste leading to environmental protection and second is the production of bio-based useful products with the help of nanotechnology. Nanoparticles have unique properties in terms of their mass-volume ratio and surface area that make them efficient for a wide variety of applications. In this study, rice husk has been used as a raw material for fabricating silica nanoparticles. Silica nanoparticles were synthesized using simple alkali extraction method. In this method, Raw material (Rice husk) was collected from local agriculture fields. They were then washed thoroughly to get rid of any dust or grain particles and sun dried at room temperature. The washed residue was then burned in muffle furnace under an inert atmosphere to produce ash which is then milled to obtain fine particles. Ash was washed with distilled water to neutralize the pH. Sample from this ash was treated with HCl to remove metallic impurities and then filtered. This filtered ash was rinsed with distilled water repeatedly and oven dried. This step was followed by burning ash in furnace to remove cabonaceous residues. The sample was then treated with caustic soda (NaOH) with continuous magnetic stirring and filtered to obtain sodium silicate. This was washed with distilled water. The sample was refluxed with H2SO4 dropwise with continuous magnetic stirring under controlled conditions and then with NH4OH to precipitate silica nanoparticles. The silica nanoparticles were then washed with double distilled water to neutralize it and then oven dried to obtain nano-silica powder. Synthesized nanoparticles were also characterized with the help of techniques like XRD, FTIR and SEM that confirmed the successful production of pure silica nanoparticles without any impurities. After that, the pot experiments were conducted with soil samples in triplicate.Silica nanoparticles (Controlled, 5%, 10% and 15% per 2Kg of soil) were added in each pot. The experiments were conducted for two weeks in which mint and barley plants were grown. Then Chemical analysis of soil sample were carried out and it includes pH, Electrical conductivity, Cations Exchange capacity, Calcium, Magnesium, phosphorus, Sulphur, sodium, Potassium, iron, Nickel, Copper, Zinc and Cadmium .Their use and effect as fertilizer in plant growth parameters were analysed in plants.

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Electrochemical Performance of Hybrid Spinel Ferrite /Carbon (Nife2o4/C) Nanocomposite Derived From Metal-Organic-Frameworks (MOF) as Electrode Material for Supercapacitor Application

Mahak Gupta[1] *, Sachin Tyagi[2], Neelam Kumari[2]
[1] *AcSIR, CSIR-CSIO,Chandigarh (India)*
[2] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India (India)*

* mahakgupta270@gmail.com

Abstract ID #NEE- 703

Electric devices and hybrid electric vehicles have raised the demand for large electric energy storage which can be fulfilled by the supercapacitor (SC). Supercapacitors possess superior properties of fast charging, high power density, and long cycle life, so are seeking eminence attention in various fields like photographic flashes, electric vehicles, power emergency actuators in airlines, wearable and foldable electronics, etc. [1–2]. In Electric Double Layer Capacitors (EDLC), carbonaceous materials employ surface adsorption to store charges whereas, in Pseudocapacitors, metal oxides and polymers use redox reactions for charge storage. Due to the usage of redox reaction phenomena for charge storage in Pseudocapacitors, the electrodes must be capable of high electrochemical activities. In this regard, Metal oxides, hydroxides, phosphides, sulphides, and Metal-organic frameworks are being used as electrode materials these days [3-5].

MOFs derived spinel ferrites which are a type of mixed metal oxides are of great interest in energy storage applications due to smaller charge activation energy and enhanced electrical conductivity as compared to other metal oxides derived from MOF [6]. Among various spinel ferrites, Ni Ferrite has been explored much due to its better electrochemical and thermal stability, enhanced redox reaction from various oxidation states, and low cost. Additionally, NiFe2O4 is non-toxic and, the precursor required for the synthesis is inexpensive and easily available [7-8]. However, agglomeration of NiFe2O4 nanoparticles during synthesis is a major drawback for energy storage applications [9]. It is important to note that, NiFe2O4 must be obtained in a consistent morphology for charge storage applications.

In present research, Ferrite/carbon (NiFe2O4/C) nanocomposite derived from surfactant-free Metal-organic frameworks (MOF) has been evaluated as electrode material for supercapacitors. The ferrite/carbon hybrid is synthesized via one step solvothermal method followed by pyrolysis for 2 hours. The thermal treatment has given rise to porous diamond shaped ferrite/carbon nanocomposite. Pyrolysis of MOF has resulted in homogeneous distribution of ferrite on carbon with lesser agglomeration which moderated the active surface area. The material synthesized at 500°C in N2 environment exhibits electric double layer capacitance (EDLC) and pseudocapacitive charge storage mechanism with the highest specific capacitance of 85.5 F g-1 at a current density of 0.25 A g-1. The high specific capacitance of synthesized material can be attributed to surface redox reaction from a large active surface area. Asymmetric supercapacitor comprised of NF500 and activated carbon has shown a high energy density of 21.31 Wh Kg-1 at a power density of 54.72 W Kg-1.

ACKNOWLEDGMENTS

The author Mahak Gupta is thankful to the DST-Inspire (IF-180134) for her research grant. The authors are thankful to CSIR-IMTECH for providing a few characterization facilities. The authors are thankful to the Director, CSIR-CSIO Chandigarh for providing full facilities in the lab.

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Composite PEDOT:PSS Films With SWCNT and Ag Nanoparticles for Solar Cell Application

Sergii Mamykin *, Tetiana Lunko, Iryna Mamontova, Olga Kondratenko, Tetiana Semikina, Volodymyr Romanyuk

V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 41, 03028, Kyiv, Ukraine (Ukraine)

* mamykin@isp.kiev.ua

Abstract ID #NEE- 718

For the fabrication of organic solar cells a heterojunction between p-type PEDOT:PSS conductive polymer and n-type crystalline silicon is used widely. Films of this polymer transmit radiation well in the spectral range of silicon photosensitivity and have good conductivity, although lower compared to ITO films. Therefore, finding ways to increase the conductivity of PEDOT:PSS films while maintaining their high transmittance is an important problem to be solved in organic photovoltaics.

One of the methods is physical doping of polymer films. The introduction of a small amount of carbon nanotubes can increase the conductivity of the polymer films without significantly affecting its transparency. Also PEDOT:PSS has a high value of the work function therefore its contact with noble metals (Ag, Au) is ohmic, which opens the possibility of improving the conductivity of PEDOT films by adding nanoparticles of these metals. In addition, it is possible to use the effects of plasmon enhancement of the electromagnetic field near metal nanoparticles, directed light scattering into the substrate, thereby increasing light absorption and reducing reflection losses.

In this work, we study an effect single wall carbon nanotubes and Ag nanoparticles admixtures in PEDOT:PSS films on their optical and electrical parameters as well as on parameters of Si-based photoconverting heterostructures. Film thicknesses and optical parameters were obtained from spectroscopic ellipsometry in the range of 0.5-5.0 eV, while electrical dc-conductivity with four-point probes method.

Composite films revealed higher conductivity compared to pure PEDOT:PSS and the corresponding solar cell structures showed higher efficiency (compared to solar cells based on PEDOT:PSS/Si). Investigation of the photoelectrical properties of such composite films made it possible to create silicon-organic solar cell heterostructures with competitive photovoltaic characteristics.

ACKNOWLEDGMENTS

The authors appreciate funding from the Ministry of Education and Science of Ukraine (Project No. 0122U001956), from the CRDF 2022 U.S.-Ukraine Alternative Energy Research Competition grant (G-202206-68887) and the IEEE program "Magnetism for Ukraine 2022", supported by the IEEE Magnetic Society under the Science and Technology Center in Ukraine (STCU) framework, project Number 9918.

Polylactide Nanocomposites with Increased Performance Properties

Andrii Masyuk *, Bozhena Kulish, Dmytro Kechur, Volodymyr Levytskyi
Lviv Polytechnic National University (Ukraine)

* masyukas@gmail.com

Abstract ID #NEE- 720

Today due to the low level of reuse of polymeric materials, the most acceptable and generally accepted direction in the development of chemistry and technology of polymeric and composite materials is the use of biodegradable polymers that are capable of controlled decomposition in environmental conditions by external factors. In this regard, the most promising is polylactide (PLA) - a biocompatible biodegradable thermoplastic polymeric material derived from renewable raw materials [1]. At the same time, the morphology and operational (tensile strength, modulus of elasticity, surface hardness, heat resistance, etc.) characteristics of polymers, in particular polylactide, significantly depend on the content of applications of different nature. Therefore, the directed action on the morphology of polylactide, in particular its additional heat treatment, and the introduction of the nucleator of the crystallization process - talc can regulate the properties of the material in a wide range. In this work, polylactide of company NatureWorks Ingeo 2500 HP, as well as nano talc filler - were used to obtain polymer composite materials. Based on the results of FTIR spectroscopic and X-ray diffraction studies, the effect of heat treatment on the supramolecular structure of polylactide and on the change in intermolecular interactions under the influence of talc was revealed. In particular, an increase in the value of the degree of crystallinity of the polylactide and a decrease in the size of the crystallites after the heat treatment process at a temperature of 120 °C for 3-10 min. The hardness of the obtained polylactide materials was studied, in particular, there is an increase in hardness due to the introduction of filler and additional heat treatment. The highest value of hardness of 242 MPa is characteristic of the heat-treated material with 2% wt. of talc. It was found that the addition of talc to the PLA and additional heat treatment contributes to a significant increase in the values of Vicat softening point of polylactide materials by 50-60 K. The greatest impact on Vicat softening point has additional heat treatment. The introduction of 2% wt. nanotalc allows you to reduce the required heat treatment time to achieve high values of Vicat softening point. There is also an increase in the modulus of deformation by 45-95% and the modulus of elasticity by 15-50% of polylactide materials under the action of filler and heat treatment, in particular, the highest values are characteristic of heat-treated samples with nanotalc content of 2% wt.

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Preparation and Characterization of Ceramic-Based Thick-Film Nanostructures for Sensor Applications

Yuriy Kostiv[1] *, Halyna Klym[1], Ivan Hadzaman[2]
[1.] *Lviv Polytechnic National University (Ukraine)*
[2.] *Drohobych Ivan Franko State Pedagogical University (Ukraine)*

* yura.kostiv@gmail.com

Abstract ID #NEE- 723

Thick-film technology is an attractive option for the fabrication of functional electroceramics due to its simplicity, cost-effectiveness, and suitability for a wide range of applications [1]. Among the different types of functional electroceramics, ceramics based on the mixed NiMn2O4-CuMn2O4-MnCo2O4 system exhibit superior performance in terms of their thermal and electrical properties. In addition, when combined with layers of humidity-sensitive nanostructured MgO-Al2O3 ceramics, they offer several advantages over other types of electroceramics.

The primary objective of this work was to fabricate and characterize the structural properties of temperature- and humidity-sensitive thick-film nanostructures. The researchers investigated thick-film temperature-sensitive elements and multilayered structures based on Cu0.1Ni0.8Co0.2Mn1.9O4 with p-type electrical conductivity, Cu0.1Ni0.1Co1.6Mn1.2O4 with p+-type of electrical conductivity, and dielectric MgO-Al2O3 (i-type). To achieve this, the humidity-sensitive thick-film layer was applied to a pre-formed temperature-sensitive layer.

It is worth noting that the fabrication of p-p+, p-p+-p, thick-film structures, and integrated temperature-humidity-sensitive p-i-p+ structures was carried out within one technological cycle. The researchers showed that the structure of humidity-sensitive thick films is prominently selected on a background of Al2O3 substrate with conductive Ag layer. The material contains shallow pores that serve as ducts for the receipt of water to nanopores, where processes of capillary condensation takes place, and also macropores that provide the effective receipt of water in the inner structure of the material from the environment.

In contrast to the microstructure of humidity-sensitive MgO-Al2O3 thick films, Cu0.1Ni0.8Co0.2Mn1.9O4 thick films contain a greater amount of macropores formed in clusters. A similar structure is also characteristic of bulk material of the same composition. Thus, the structural features of ceramics can be transformed into thick films of similar compositions. The use of ceramic with a spinel structure as the main output component for the preparation of thick films provided the density of the multi-layer structure and the component for the production of thick films, provided the density of the multi-level structure and contact of their layers.

Overall, the results of this work demonstrate that the fabrication of thick-film nanostructures based on ceramics of mixed compositions is a promising area of research for the development of functional ceramics. The thick-film technology used in this study offers a simple, cost-effective, and versatile approach to fabricating these materials for a wide range of applications, including sensors, actuators, and energy harvesting devices. Future work could focus on optimizing the structural properties of these materials to improve their performance and broaden their potential applications.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Education and Science of Ukraine (Project No 0122U000807).

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Computational Fluid Dynamics (CFD) Approach Towards Atomic Layer Deposition (ALD) Process Optimization

Michal Pecz[1*], Boris Hudec[2]
[1] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 841 04 Bratislava, Slovak Republic (Slovakia)*
[2] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

* elekpecz@savba.sk

Abstract ID #NEE- 725

Ever growing need for better batteries resulted in constant pressure on raising energy densities and lowering costs. One way of achieving this was reached by covering their cathodes by protective ultra-thin films.

LiFePOx (LFPO) cathodes are essential for working of Li-ion batteries, due their great porosity and ability to store charge. To prevent degradation and improve capacity, multiple layers of Al2O3 were deposited on most of surface with Atomic Layer deposition (ALD)

Computational Fluid Dynamics (CFD) with Ansys Fluent and Autodesk CFD were conducted to optimise reaction parameters in pursuit of better coverage of the highly porous cathode material with high specific surface and optimising the reaction time, mainly important in industrial applications. [1]

It was discovered [2] that ideal concentration of reactant was around 2% balancing the waste and the speed of reaction. Al2O3 thin films were grown using Beneq TFS-200 equipment, with reaction of Trimethylaluminium (TMA) and water vapour.

Our work simulated effects of changing geometry, internal pressure, temperature from 100 °C- 300 °C, and pulse times, multiple flow, with many different border conditions.

ACKNOWLEDGMENTS

This work was supported by the VEGA project no. 2/0162/22, "Ultra-thin conformal surface coatings of complex-morphology structures for improving battery performance using atomic layer deposition".

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Hydrogen Storage in Ca-Decorated Doped Germanene: A DFT Study

Alvaro Miranda[1] *, Akari Narayama Sosa[2, 2], Brandom Jhoseph Cid[1], María Isabel Iturrios[3], Luis Antonio Pérez[4], Miguel Cruz-Irisson[1]

[1] *Instituto Politécnico Nacional, ESIME-Culhuacán (Mexico)*
[2.] *Benemérita Universidad Autónoma de Puebla, Instituto de Física (Mexico)*
[3.] *Instituto Politécnico Nacional, CECYT 8 Narciso Bassols (Mexico)*
[4.] *Instituto de Física, Universidad Nacional Autónoma de México (Mexico)*

* amirandad@ipn.mx

Abstract ID #NEE- 734

Germanene is a two-dimensional nanomaterial that has been successfully synthesized. In addition, they have been studied for potential energy storage and sensing applications [1-3]. In this work, we have studied the capacities hydrogen storage of Ca-decorated X-doped (X = B, Al, and Ga) germanene. Numerical results show a strong binding between Ca metal atom and doped-germanene, where metal atom adsorbed on doped-germanene are energetically favorable, therefore avoid to formation of metal clusters. Ca-decorated systems offers between 0.16 and 0.17 eV/H2 for the adsorbed hydrogen molecules and a gravimetric hydrogen storage capacity between 6.88 and 7.37 wt% achieving technical targets of the United States Department of Energy. The desorption energy of the 5H2 Ca-decorated doped germanene are achieved between 0.08 eV and 0.11 eV, the desorption temperature between 116 K and 117 K, and finally the desorption time in the order of nanoseconds under ambient temperature situations. The Ca-decorated doped germanene systems could be suitable for hydrogen storage changing temperature or pression.

ACKNOWLEDGMENTS

This work was partially supported by multidisciplinary project IPN-SIP 2023-2274 and UNAM-PAPIIT IN109320. Computations were performed at the supercomputer Miztli of DGTICUNAM (Project LANCAD-UNAM-DGTIC-180). B.J.C. would like to thank CONACYT and BEIFI-IPN for their financial support. A.N.S. thanks CONACYT for her scholarship through the program "Estancias Posdoctorales por México – Modalida 1".

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Ultrathin Atomic Layer Deposited Zno Films Improves Perfpormance of the Silicon/Graphite Anode For Li-Ion Batteries

Karol Frohlich[1] *, Prangya Parimita Sahoo[1], Alper Güneren[2], Boris Hudec[3], Miroslav Mikolášek[4], Ahmed Nada[1], Magdalena Precnerova[1, 5], Matej Mičušík[6]

[1.] *Centre For Advanced Materials Application CEMEA, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava (Slovakia)*

[2.] *Institute of Inorganic Chemistry SAS (Slovakia)*

[3.] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[4.] *Institute of Electronics and Photonics, Slovak University of Technology, SK-841 04 Bratislava (Slovakia)*

[5.] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava (Slovakia)*

[6.] *Polymer Institute of Slovak Academy of Sciences (PI SAS) (Slovakia)*

* karol.frohlich@savba.sk

Abstract ID #NEE- 737

Batteries as efficient energy storage devices became highly demanded in modern human society. Since the commercial emergence of Li-ion batteries by SONY in 1991 they have found broad use in electronics, mobile phones, portable computers, automotive industry, and energy storage [1, 2].

During Li-ion battery operation, a solid-electrolyte interphase (SEI) is formed on the surface of the electrodes as a product of the electrolyte reduction [3]. While SEI is essential for successful operation of lithium-battery systems, its uncontrolled evolution can be critical when charging by high currents and can cause failure. In our contribution we show, that protective surface coating of the silicon/graphite anode can control growth of the SEI and consequently, enhance performance of Li-ion batteries.

The silicon-graphite based anode was prepared by mixing 80 wt% silicon-graphite (ball milled at 20:80 silicon/graphite weight ratio), 10 wt% of carbon black, and 10 wt% of sulfonated-alginate as a binder. Ultrathin protective ZnO films were prepared by atomic layer deposition (ALD) on the silicon/graphite anode. The films were grown at the temperature of 100 °C in conditions adapted for growth on porous substrates. The thickness of the ZnO films was in the range up to 40 ALD ZnO cycles (4 nm).

Batteries with silicon/graphite anode were tested in a coin-like configuration using LiPF6 dissolved in ethylene carbonate/diethyl carbonate as an electrolyte and Li metal as a counter electrode. Charging/discharging experiments revealed that the discharge capacity of the silicon/graphite anodes covered by ZnO films exhibited significantly improved rate capability in particular for the c-rates 1 and 2 (high charging currents). Electrochemical impedance spectroscopy unveiled lower value of the SEI layer and charge transfer resistances for the anodes covered by ZnO films compared to the unprotected pristine anode. The results of the electrochemical impedance spectroscopy were confirmed by X-ray photoelectron spectroscopy indicating different chemical composition of the SEI layer for the ALD-protected and unprotected anodes after charging/discharging cycling.

The results demonstrate that ALD ultrathin ZnO layers can effectively protect the silicon/graphite anode. Charging/discharging experiments revealed enhanced rate capability of the electrodes covered by ALD films particularly at high charging/discharging rates. Protection of the electrodes surface by ALD ultrathin films seems to be an efficient way for control and stabilizing of the SEI layer and, consequently, achievement of improved Li-ion battery performance.

ACKNOWLEDGMENTS

This study was performed during the implementation of the project Building-up Centre for advanced materials application of the Slovak Academy of Sciences, ITMS project code 313021T081 supported by Research & Innovation Operational Programme funded by the ERDF. The authors acknowledge support of the projects APVV-19-0461.

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Ionogel Electrolytes Based on Hexagonal Boron Nitride Nanoplatelets for Lithium-Ion Batteries

Woo Jin Hyun*
Guangdong Technion – Israel Institute of Technology (China)

* woojin.hyun@gtiit.edu.cn

Abstract ID #NEE- 742

Ionogels, also known as ion gels or ionic liquid gels, are composite solid-state electrolytes, in which ionic liquids are immobilized by a gelling solid matrix. Ionic liquids offer several advantages as an electrolyte solution, including nonflammability, negligible vapor pressure, and high thermal stability. Moreover, combining ionic liquids with a gelling solid matrix leads to a solid-state electrolyte that is mechanically robust yet flexible without leakage problems, rendering it promising for flexible electronics and energy storage [1]. However, the key limitation of ionogels has historically been their weak mechanical properties, resulting in poor structural integrity. In this talk, a novel ionogel will be introduced based on exfoliated hexagonal boron nitride (hBN) nanoplatelets, achieving desirable mechanical and electrochemical properties (storage modulus > 1 MPa, room temperature ionic conductivity > 1 mS/cm) simultaneously [2]. hBN possesses several desirable attributes as a solid matrix material, including electrically insulating character, chemical inertness, thermal stability, and mechanical robustness. In addition to these intrinsic advantages, the exfoliated hBN nanoplatelets significantly enhance the mechanical strength of ionogels without compromising electrochemical properties, compared to conventional bulk hBN microparticles. This talk will discuss the mechanical and electrochemical properties of hBN ionogel electrolytes, and will also show their applications for high-voltage and fully-printed solid-state lithium-ion batteries [2–4].

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Novel Catalysts for Water Splitting: Strategies for Performance Enhancement

Tofik Ahmed Shifa[1]*, Kassa Belay Ibrahim[1], Alberto Vomiero[2], Elisa Moretti[1]
[1] *Ca'foscari university of Venice (Italy)*
[2] *Foscari University of Venice (Italy)*

* tofikahmed.shifa@unive.it

Abstract ID #NEE- 745

The generation of clean energy from water electrolysis is a feasible solution to overcome the problems of energy crisis. However, this viable route depends on the utilization of Pt, which is scarce and expensive. Designing catalysts entirely based on Earth abundant materials is, therefore, the way forward. In this regard, 2D materials (layered or non- layered), and transition metal phosphides have got copious attention. [1,2] Here, we present strategies to enhance the catalytic (electrocatalysis, photocatalysis) performance of these materials giving a particular emphasis for transition metal chalcogenides (WS2, CuS, etc), transition metal phosphorus trichalcogenides (MPX3; X=S,Se), non-layered Cr2S3 and nickel phosphides. We discuss the advantages of these materials for catalysis and the different routes available to tune their electronic states and active sites. Experimental results show that doping and hybrid material formation play a significant role in optimizing the free energy of hydrogen adsorption and desorption on the vertically oriented nanosheets of WS2. Another compelling issue in this research area is about solving the sluggish kinetics of the other half reaction (i.e OER) in water splitting catalysis. It has remained a bottleneck in realizing efficient performance. In this regard, nickel phosphide has an excellent track of performance.[3] We also discuss the mechanism behind the very good performance of Ni5P4 and CrOx-CuS toward electro-catalysis of OER. The metal phosphides or sulfides are not the true catalysts, rather in-situ generated metal oxides at the vicinity of phosphides/sulfides are. Moreover, We highlight the emerging layered MPX3 (M= Mn, Ni, Fe, Cu/In)[4] nanosheets as promising materials in sacrificial agent-free photocatalytic water splitting under simulated Sun light (AM 1.5G) illumination.

ACKNOWLEDGMENTS

The authors would also like to acknowledge Ca'Foscari university of Venice for hosting the Marie Curie fellowship of Dr.Tofik Ahmed Shifa. We would also like to thank HPC2N (Tetralith) for the allocation of high-performance computing time and resources through the Swedish National Infrastructure for Computing (SNIC). This work has been carried out within the agreement "Convenzione operativa per collaborazione scientifica tra CNR ISM e Dipartimento di Scienze Molecolari e Nanosistemi Universit` a Ca ` Foscari Venezia (Prot.n. 709, 14/04/2021)". Partial support through the project EUROFEL-ROADMAP ESFRI is also gratefully acknowledged."

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Correlation of Electrophysical and Mechanical Properties of Polymer Nanocomposites Based On Epoxy Resin With Carbon Fibers

Oksana Lisova[1]*, Stanislav Makhno[2, 3], Ruslana Mazurenko[1], Sergey Prokopenko[1], Yurii Sementsov[2, 3], Mykola Kartel[1]

[1.] *Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine (Ukraine)*
[2.] *Ningbo University of Technology, No 55-155 Cui Bai Road, Ningbo, 315211 (China)*
[3.] *Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute, Kechuang building, N777 Zhongguan road, Ningbo, 315211 (China)*

* oksana.garkusha@gmail.com

Abstract ID #NEE- 748

Polymer composites reinforced with carbon fibers are widely used in various industries due to excellent mechanical and structural properties, chemical stability, etc. The fibrous component of the composite should be evenly distributed throughout the volume of the polymer, forming a branched network, namely, a continuous percolation cluster. The uniformity of the distribution of the conductive filler in the polymer matrix is traditionally evaluated using electrophysical research methods, and it is also possible to evaluate the important operational characteristics of composites without performing additional research, which is shown in this work.

Using for example of both epoxy resin–carbon fiber (ER-CF) and epoxy resin–carbon fiber on glass fabric (ER-CF-GF) systems, it was established a correlation of the electrophysical and mechanical properties of polymer composite systems by the method [1] at the conductive filler concentration in the area percolation threshold.

The real and imaginary components of the complex dielectric permittivity in the microwave range for polymer composites of both systems reached high values (up to 40) at CF ~ 0.01 volumetric content, due to the effective interaction of the system components and the filler's uniform distribution in the polymer matrix. The nonlinear character of the increase of the values of ε', ε" in both systems with the increasing volume content of the CF was observed.

The electrical conductivity at low frequencies for ER-CF-GF and ER-CF systems in the range of CF content 0-0.12 of the volume fractions changed symbatically. A sharp increase in electrical conductivity at a CF content in the polymer of 0.003–0.005 vol. fractions was observed and may be explained a percolation transition in the systems. The electrical conductivity results were analyzed using percolation theory and corresponding percolation thresholds were determined, for the ER-CF-GF composites is $\phi c = 0.0023$ (t=2.1), for the ER-CF composites is $\phi c = 0.0032$ (t=1.83).

The dependences of the relative bending strength on the volumetric content of explosives for both systems had a parabolic shape. The maximum value of the relative tensile strength is observed for the content of CF, slightly higher than the value of ϕc for each system. Correlation of mechanical properties and electrical conductivity at low frequencies in the region of the percolation threshold was established. The bending strength has optimal indicators in the region of 0.001-0.005 vol. of the filler after the percolation threshold.

It is possible to predict the mechanical properties of polymer nanostructured composites with conductive fillers based on the results of electrophysical studies, which provides prospects for optimizing the electrophysical and mechanical characteristics of composites with different types of fillers.

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Lithium Iron Phosphate Cathodes Protected By Ultrathin Alumina Films By Atomic Layer Deposition

Prangya Parimita Sahoo[1] *, Boris Hudec[2], Miroslav Mikolášek[3], Magdalena Precnerova[1, 4], Matej Mičušík5, Karol Frohlich[1]

[1] *Centre For Advanced Materials Application CEMEA, Slovak Academy of Sciences, Dúbravská cesta 9, 845 11 Bratislava (Slovakia)*

[2] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská Cesta 9, SK-841-04 Bratislava (Slovakia)*

[3] *Institute of Electronics and Photonics, Slovak University of Technology, SK-841 04 Bratislava (Slovakia)*

[4] *Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, 84104 Bratislava (Slovakia)*

[5] *Polymer Institute of Slovak Academy of Sciences (PI SAS) (Slovakia)*

* prangya.sahoo@savba.sk

Abstract ID #NEE- 764

Lithium-ion rechargeable batteries have become an integral part of our life. Different classes of oxide materials including LiCoO2 (LCO), LiFePO4 (LFP), LiMn2O4 (LMO), and Li1.05Ni0.33Mn0.33Co0.33O2 (NMC), LiNi0.8Co0.15Al0.05O2 (NCA) have been explored for their utilization as cathodes in LIBs.

The LiFePO4 (LFP) cathode has a theoretical specific capacity of 170 mAh/g and is stable, safe, and environmentally benign. Li-ion batteries with LFP cathodes have a long cycle life with excellent charging/discharging performance. In our contribution, we show that the surface modification of the LFP cathode using ultrathin alumina films grown by atomic layer deposition (ALD) improves Li-ions charge transfer and rate performance of the Li-ion in half-cell and full-cell configurations.

The half cells used in our study consisted of Li anode and LFP electrodes as cathodes whereas for full cell configuration graphite and LFP electrodes were used as anode and cathode, respectively. The LFP electrode had a thickness of 70 µm and the average LFP particle size was 2 µm(commercial NANOMYTE BE-60E (NEI Corp.).

Ultrathin Al2O3 films were grown on LFP cathodes by atomic layer deposition (ALD) at 100 °C using trimethyl aluminum and water vapors. The growth rate of the Al2O3 films was 0.1 nm/cycle. The thickness of the ALD layers depends linearly on the number of ALD cycles and for 2 to 50 cycles and ranges from 0.2 to 5 nm.

Galvanostatic charging/discharging experiments were performed to evaluate the rate capability of the electrodes. Pristine and Al2O3 coated LFP electrodes were laser cut to 18 mm diameter circular electrodes, inserted in the electrochemical test cells PAT-Cell (EL-CELL), and tested using PAT-Tester-x-8 analyzer. LFP with Al2O3 protecting layers was compared to the pristine LFP electrode in half-cell and full-cell configurations. The electrodes protected by Al2O3 film always had better rate capability than the pristine sample. High-temperature charging/discharging measurements confirmed better cycling stability of the Al2O3-coated cathodes.

Investigation of the rate capability fading using electrochemical impedance spectroscopy revealed a gradual increase of the Nyquist plot semicircle diameter as a function of cycles. Results obtained by electrochemical characterization are compared to the X-ray photoelectron spectroscopy and scanning electron microscopy performed on samples before and after galvanostatic charging/discharging measurement.

Al:$SrTiO_3$@Fe_2O_3@void@SiO_2 Nanoreactors for Efficient Visible Light-Driven Photocatalytic Water Splitting

Ioana Radu[1], Daniel Gherca[2] *, Georgiana Andreea Bulai[3], Adrian Iulian Borhan[1], Aurel Pui[1]
[1] *"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, Carol I nr. 11 Blvd., Iasi 700506, Romania (Romania)*
[2] *National Institute of Research and Development for Technical Physics, 47 Mangeron Boulevard, Iasi 700050, Romania (Romania)*
[3] *Integrated Center of Environmental Science Studies in the North-Eastern Development Region (CERNESIM), Department of Exact and Natural Sciences, Institute of Interdisciplinary Research, Alexandru Ioan Cuza University of Iasi, 700506 Iasi, Romania (Romania)*

* daniel_gherca@yahoo.com

Abstract ID #NEE- 785

At the forefront of renewable energy research, scientists have turned their attention to the fascinating world of nanoheterostructures [1]. In particular, core-multi shell nanoheterostructures have shown great promise for their ability to efficiently split water into hydrogen and oxygen [2]. These types of heterostructures consist of a core material (Al:SrTiO3) surrounded by a shell (Fe2O3) with a void space in between of SiO2 outer shell, acting as a hollow structure for enabling multiple reflections and scattering of incident light inside shells, thus prolonging the path of light to enhance its photocatalytic activity. However, the optimal composition for efficient water splitting has remained a topic of debate [3]. In the present study, we aim to go far beyond state of the art through full exploitation of core/shell@void@shell 3D nanoreactors (Al:SrTiO3@Fe2O3@void@SiO2) based on tuning morphologies, utility and functionality of their nano-constituent building units to enhance the activity demands of photocatalytic applications, particularly for water splitting. By demonstrating the importance of each constituent in the design of such nanoheterostructures for efficient water splitting, our findings could pave the way for the development of more efficient and cost-effective renewable energy technologies [4]. The preapration of the nanomaterial is obtained by a simple, economical and environmentally friendly method that involved the assembly of oxyhydroxide over colloidal perovskite suspension following the SiO2 additions and thermal treatment. A coprehensively formation mechanism is proposed based on systematic investigation of the synthetic process. In-depth caracterization of structural, optical and morphological properties of the prepared core/shell@void@shell 3D nanoreactors (Al:SrTiO3@Fe2O3@void@SiO2) was investigated using a series of complementary analytical techniques, such as XRD, FE-SEM and soft XAS in both total electron yield (TEY) and fluorescence yield (TFY). The photocatalytic water splitting activities were carried out under the visible light irradiation at room temperature and evolved gases being in-situ quantified using H2/O2 microsensors. Furthermore, this study highlights the potential of core/shell@void@shell 3D nanoreactors (Al:SrTiO3@Fe2O3@void@SiO2) as a promising platform for clean and sustainable energy production.

ACKNOWLEDGMENTS

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-1385, within PNCDI III.

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Al:$SrTiO_3$/CoOOH Core-Shell Nanoarchitectures: a Promising Framework for Highly Efficient Adsorption of Tropaeolin 00 Dye and Oxacillin from Wastewater

Ioana Radu[1] *, Daniel Gherca[2], Adrian Iulian Borhan[1], Georgiana Andreea Bulai[3], Daniela Dirtu[1], Alin Constantin Dirtu[1], Aurel Pui[1]

[1] *"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, Carol I nr. 11 Blvd., Iasi 700506, Romania (Romania)*

[2] *National Institute of Research and Development for Technical Physics, 47 Mangeron Boulevard, Iasi 700050, Romania (Romania)*

[3] *Integrated Center of Environmental Science Studies in the North-Eastern Development Region (CERNESIM), Department of Exact and Natural Sciences, Institute of Interdisciplinary Research, Alexandru Ioan Cuza University of Iasi, 700506 Iasi, Romania (Romania)*

* oanaradu833@gmail.com

Abstract ID #NEE- 786

Adsorption process has emerged as an essential technique to remove harmful pollutants (dyes and antibiotics) from wastewater, as it provides an effective and economical solution to tackle environmental pollution [1]. Core-shell nanocomposites are advanced materials that have unique surface properties, such as high surface area and chemical stability, making them ideal for adsorption applications [2]. They have gained significant attention due to their ability to effectively remove various pollutants, including heavy metals, dyes and active pharmaceutical ingredients compounds [3]. Recent studies have shown that core-shell nanocomposites have high adsorption capacities for various antibiotics [4], however, there is a need to investigate the adsorption performance by developing specific-tailored adsorption process based on the nanomaterials properties to efficiently remove these pollutants from wastewater. In this study, we investigate the adsorption properties of Al:SrTiO3/CoOOH nanocomposite for the removal of harmful dyes and antibiotics from water. The nanocomposite was synthesized using a simple and cost-effective method and characterized using various techniques (FTIR, XRD, SEM, DRS, BET). The results show that the nanocomposite has a high degree of adsorption capacity for both dyes and antibiotics, making it a promising material for water treatment applications. The adsorption capacity of the Al:SrTiO3/CoOOH nanocomposite was found to be 11.75 mg/g and 3.87 mg/g for Tropaeolin OO dye (6 mg/L) and Oxacillin (5 mg/L) respectively. The high adsorption capacity of the core-shell nanocomposite can be attributed to its own properties: the shell layer (CoOOH) provides a large number of active sites for adsorption, while the core (Al:SrTiO3) enhances the chemical reactivity and stability of the material. This study provides valuable insights into the use of core shell nanocomposites for the removal of harmful pollutants from water, which can have significant implications for environmental and public health. The results of this study can provide a basis for future research in the development of advanced materials for wastewater treatment.

ACKNOWLEDGMENTS

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P4-ID-PCE-2020-1385, within PNCDI III.

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Synthesis and Characterization of Ti-MOF Based Magnetically Retrievable Composite for the Selective Detection of Enteropathogenic E.Coli

Saloni Sharma[1] *, Gurjeet Kaur[1], Manoj Nayak Kumar[2], Akash Deep[3]

[1] *AcSIR, CSIR-CSIO,Chandigarh (India)*

[2] *CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C Chandigarh (India)*

[3] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India (India)*

ssaloni007@gmail.com

Abstract ID #NEE- 787

Food safety has emerged as an important global issue as it impacts the wellbeing of individuals as well as nations. Food borne illness from enteropathogenic E.coli is a significant health concern as it causes infantile diarrhoea worldwide which corresponds to high rate of morbidity and mortality among children. The conventional methods of pathogen detection are complex, laborious and time consuming. Hence, biosensors are emerging as a potential platform for the early detection of food borne pathogens [1,2]. This work presents a unique combination of nano-sized magnetite nanoparticles (Fe3O4), surface functionalized with a silica shell and immobilised on Ti- MOF framework. The Fe3O4 nanoparticles have been extensively used due to their magnetic properties, biocompatibility and minimal side effects [3]. The silica shell around the magnetic core provided water stability to the core-shell nanostructure. Ti-MOF provided high surface area and stable optical response in the selective detection of E.coli. For ensuring the selectivity of the biosensor, the anti- E.coli monoclonal antibody was immobilized through EDC-NHS carbodiimide crosslinking mechanism. The Ti-MOF@Fe3O4@SiO2 magnetic composite was characterized by various analytical techniques such as XRD, FESEM, FTIR, PL and UV spectroscopy. The optical response against E.coli was recorded through Photoluminescence Spectroscopy. The detection results showed high sensitivity and specificity. The bacteria attached magnetic framework composite was magnetically recyclable highlighting its application in water treatment. Therefore, the MOF based core-shell magnetic platform was effective in the biosensing and removal of food borne pathogen E.coli.

ACKNOWLEDGMENTS

The authors would like to acknowledge the research fellowships provided by CSIR-CSIO India. This research work was conducted by the project grant funded by CSIR-CSIO Chandigarh under project MLP-2006. In addition, the authors are very thankful to the Director of CSIR-CSIO, Chandigarh for providing all the necessary facilities.

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The Impact of Chemical Activation on the Structure and Surface Characteristics of Kaolin

Antonina Bondarieva *, Viktoriia Tobilko

National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)

a.i.bondarieva@gmail.com

Abstract ID #NEE- 799

Modifying the structure and surface properties of clay minerals allows for expanding their range of applications. Achieving this uses a range of physical and chemical modification methods [1]. Chemical activation is one of the most straightforward methods to implement in industrial conditions. For example, many studies have shown the potential of chemical activation of montmorillonite through its alkaline and acid treatment. However, the possibility of chemical activation of other types of clay still needs more study.

With this aim, the object of this study is kaolin (Glukhovets deposit, Ukraine). Chemical activation was carried out using hydrochloric acid of different concentrations. The temperature of acid activation was also varied.

Due to its low reactivity, natural kaolin exhibits weak reactions with acid [2]. Therefore, in the first step of work, we obtained an active form of kaolin, metakaolin (mK), by high-temperature treatment (600°C) in a muffle furnace. Next, a suspension of mK was prepared in an HCl solution with a liquid-to-solid ratio of 10:1. Acid activation was carried out using a lab condenser for 4 hours. After that, the suspensions were cooled to room temperature, repeatedly washed with distilled water, and filtered using a vacuum. The obtained samples were dried at 80°C to a constant weight.

The study the effect of the chemical activation of kaolin on the structure and properties of its surface, the following methods were used: X-ray powder diffraction (XRD), low-temperature nitrogen adsorption/desorption method, scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM/EDS), FTIR spectroscopy, and conductivity measurements.

With a decrease in the intensity of characteristic reflections of kaolin in X-ray diffraction patterns and an increase in the width of the IR bands of thermally activated samples, it can be concluded that the formation of mK was successful. The results of low-temperature N2 adsorption/desorption indicate a dependence of the specific surface area of the obtained materials on the concentration of the acid used for activation. Specifically, an increase in the initial HCl concentration increases the specific surface area of the samples. Additionally, chemical activation performed at 80 °C allowed for further enhancement of the specific surface area (from 61 m2/g to 140 m2/g) compared to chemical activation performed at 60 °C under the same initial concentration of hydrochloric acid. Changes in surface morphology and elemental composition of acid-treated samples compared to the starting mineral were traced through SEM/EDS analysis.

Therefore, acid activation of thermally treated kaolin significantly improves its physicochemical properties. In future studies, it would be useful to investigate the potential use of the obtained materials for environmental protection.

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Optical and Photoelectric Properties of Cdte:In Thin Films Deposited By PVD Technique

Ivanna Vakaliuk[1] *, Rostyslav Yavorskyi[1], Bohdana Naidych[1], Lyubomyr Nykyruy[1], Lilia Katanova[1], Oksana Zamurueva[2]

[1] *Vasyl Stefanyk Precarpathian National University (Ukraine)*
[2] *Lesya Ukrainka Volyn National University (Ukraine)*

ivanna.maliarska@pnu.edu.ua

Abstract ID #NEE- 804

Modern fossil resources, such as oil, coal and natural gas require significant costs at the stage of extraction and conversion into electricity through the use of complex technologies [1,2]. The mining process is accompanied by a harmful impact on the environment, and it takes an extremely long time to restore them. Therefore, the search for alternative sources of energy has become extremely relevant and continues to be the object of research by scientists and power engineers all over the world [3]. The use of renewable technologies makes it possible to create an energy system that will contain a minimum of carbon at an affordable price. Photovoltaic panels are currently the most commercialized solar energy technology, covering a large part of global markets [4]. An alternative to silicon is currently cadmium telluride (CdTe). The main advantages are strength, chemical stability and suitability for application to a variety of surfaces using a wide range of methods depending on the end needs and technology [5]. The doping can control the optical, electrical, and mechanical properties of CdTe thin films. The elements of the first and fifth groups of the periodic system play the role of acceptors, and the third and seventh – donors.

Physical vapor deposition method was used to synthesize thin films using glass and (100) silicon substrates at consistent evaporation and substrate temperatures. The same production circumstances (different sample thicknesses) were used to build CdTe:In thin film nanostructures on silicon substrates. The previously obtained indium doped cadmium telluride has an evaporation temperature of TE = 550°C. The deposition temperature on the substrate was TS = 200°C. The thickness of the condensate ranges from 540 to 2835 nm, was determined using the Bruker Dektak XT profilometer and predefined by setting the time of deposition in range (30 – 570) sec.

The optical properties indicate smooth films with nanoparticles size on surface for both thin and thick films of CdTe:In. An analysis of the optical properties was performed using the Swanepoel method. Hence, the basic properties of the films such as refractive index, film thickness, absorption coefficient and optical conductivity are determined. The optical transparency is observed in the short infrared radiation.

ACKNOWLEDGMENTS

This study was supported by the Ministry of Education and Science of Ukraine as the project for young scientists "High-efficiency hybrid thin-film solar cells for energy security and sustainable development" (0123U100226).

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Comparing Heat Transfer Rates of Water Based Nanofluids Using a Figure of Merit

Tetiana Rymar[1*], Myroslava Kazmiruk[2]

[1] *Lviv Polytechnic National University (Ukraine)*
[2] *State Inspectorate for Energy Supervision of Ukraine (Ukraine)*

tetiana.i.rymar@lpnu.ua

Abstract ID #NEE- 816

In order to improve the safety of nuclear power plants, it is proposed to use the nanofluids as a heat carrier in heat exchangers for scheduled and emergency cooling of the NPP power unit. The intensity of heat exchange depends on the thermo-physical properties of heat carriers, and these properties depend on the nature of the heat carrier [1 - 3]. The addition of nanoparticles to the base heat carrier significantly increases its viscosity, which is accompanied by an increase in hydraulic resistance and an increase in pumping power. In this work, the influence of the nature of water-based nano-heat carriers and the content of nanoparticles in the heat carrier on some figure of merit (FOM) is studied. The analysis of the numerical values of FOM makes it possible to evaluate the efficiency of the use of heat carriers. The analysis of the quantitative assessment of heat transfer efficiency of aqueous dispersions of nanoparticles of metal oxides (Al2O3; TiO2; SiO2; ZnO; CuO) was performed in the work. The results showed that the heat carrier with CuO nanoparticles has a higher Muromtsev number (Mo), that is, it has good thermo-physical parameters for heat exchange intensification. Also, the coolant with CuO nanoparticles is characterized by the better efficiency and economy indicators, because it has the lowest value of FOMpumping. A heat carrier with Al2O3 nanoparticles requires the smaller layer of thermal insulation to reduce heat losses, as it has the lowest value of FOMheat losses. The results of the theoretical research can be used to intensify the heat exchange of power systems that use the heat carriers with an average temperature of 75 °C.

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Ultrafast Carrier Dynamics of Nanomaterials to Manipulate Light Harvesting

Amitava Patra[1,2*]

[1] *Institute of Nano Science and Technology, Knowledge City, Sector 81, Mohali 140306 (India)*
[2] *School of Materials Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032 (India)*

amitavapatra.patra@gmail.com

Abstract ID #NEE- 822

Nanomaterials-based light-harvesting systems have been the research subject because they can generate exciton after photoexcitation. A deep understanding of hot carrier (HC) dynamics is crucial to improving the performance of optoelectronic devices by reducing thermalization losses. Here, we investigate the carrier dynamics, energy transfer, and charge carrier dynamics of 2D nanoplatelets, perovskite nanocrystals, and conjugated polymer nanoparticles.1-6 Ultrafast spectroscopic investigations provide direct insight into the impacts of electron and hole transfer at the interface of hybrid materials for optoelectronic applications. The fundamental knowledge of these photophysical processes is crucial for developing efficient light-harvesting systems.

ACKNOWLEDGMENTS

TRC-DST

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Tuning Optoelectronic Properties of 0-Dimensional Nanostructures Toward High-Efficiency Luminescent Solar Concentrators

Kassa Belay Ibrahim[1], TOFIK AHMED SHIFA[1], Elisa Moretti[1], Alberto Vomiero[2]*

[1] *Ca'foscari university of Venice (Italy)*
[2] *Foscari University of Venice (Italy)*

alberto.vomiero@unive.it

Abstract ID #NEE- 831

Luminescent solar concentrators (LSCs) are an old class of devices based on semitransparent windows, in which luminophores are embedded in a transparent matrix. The luminophores can absorb and re-emit solar light and are able to generate electric power by collecting the re-emitted light at the borders of the slab. In the past, lab-to-fab transition of such devices was impeded by intrinsic limitations of the luminophores in terms of low quantum yield, strong resorption due to small Stokes shift, low optical and photoconversion efficiency of the final device. In the last years, a renaissance of such devices has been driven by the development of new 0-dimensional nanostructures [1], with tunable optical properties, which can guarantee good performance of LSCs. Specifically, high quantum yield can be obtained; resorption losses can be limited by modulating the Stokes shift; final color of the window can be tuned by tuning light absorption properties; UV and IR parts of solar spectrum can be exploited without affecting window transparency. We will give examples of different 0-dimensional systems, which have been developed toward high efficiency LSCs, among which inorganic quantum dots [2,3] and carbon dots [4]. Several strategies will be illustrated to tune the optoelectronic properties of the luminophores, including doping, core-shell structuring, and surface treatments.

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Chitosan Cross-Linked Polymer Based Edible Coatings As Tool to Improve Quality And Shelf-Life of Fresh Fruits

Raj Rani[1] *, Poonam Kumari[1], Disha disha[2], Manoj Kumar Patel;[2], Manoj Nayak Kumar[2]

[1] *Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India (India)*
[2] *CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C Chandigarh (India)*

rajrani211996@gmail.com

Abstract ID #NEE- 848

Globally, food security and safety have become a major challenge. Researchers are searching for natural components to develop biologically active packaging materials. In this regards, consumers and researchers are now more focused on improving the quality and safety of food as a result of the rejection of chemical additives [1-3]. The purpose of this work is to produce and evaluate potential edible packaging films based on chitosan cross-linked polymer by Free Radical Polymerization (FRP) to enhance chitosan's antimicrobial activity. Chitosan is a natural, renewable resource-based polymer that is biodegradable and biocompatible. It has several uses in a variety of industries, including the production of edible coatings and films. Although chitosan contains antibacterial and antifungal properties that make it suitable for food protection, its usage are restricted by the material's poor mechanical strength and high gas and water vapour permeability. Sincere efforts are being further made to improve the efficiency of edible films using biocompatible functionalize polymer. The mechanical performance of the crosslinked polymer network is improved with an increase of the mechanically and how permeable they are to gases and water vapour. X-ray diffraction (XRD) and scanning electron microscopy have been used to evaluate the miscibility and morphology of the film. The thermal property of the chitosan-polymer film has been carried out by differential electron microscopy (DSC) and Thermogravimetric analysis (TGA). These polymer have unlocked a new dimension for enhancing functional properties of polymer/chitosan-based films. These functional compounds are now emerging as an important component of edible films/coatings for prolonging shelf-life of fruits and vegetables. The antibacterial activity will be explored against the model bacterium such as S.aureus and Escherichia coli. This cross-linked chitosan-polymer film is an ideal material for food packaging applications.

ACKNOWLEDGMENTS

The authors would like to thank UGC for financial support. The authors are thankful to CSIR-Central Scientific Instruments Organisation, Chandigarh, India for providing the analytical facilities to conduct the research work.

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Acetylene Gas Pyrolyzed Carbon Structures for the Aqueous Supercapacitor Applications

Vishal Shrivastav[1*], Wojciech Nogala[1], Shashank Sundriyal[2]

[1] *Institute of Physical Chemistry Polish Academy of Sciences (Poland)*

[2] *Regional Centre of Advanced Technologies and Materials, Czech Advanced Technology and Research Institute, Palacký University, Olomouc (Czech Republic)*

vshrivastav@ichf.edu.pl

Abstract ID #NEE- 850

The demand for effective energy storage devices has increased tremendously along with the electrification of gadgets. The current state of renewable energy storage devices is being addressed and improved by a number of EU programs, including Batteries 2030+ and ERA net+ energy. Supercapacitors have a high power density and can charge and discharge much faster than batteries, which is a crucial requirement for electric vehicles and several other devices. In this work, we have synthesized a nanosized spherical interconnected carbon structure by the rapid pyrolysis of acetylene gas. The obtained carbon, when analyzed through the SEM showed the spherical type morphology interconnected with each other. The XRD pattern of the carbon showed the amorphous structure of the carbon. The carbon is further used as an electrode material for aqueous supercapacitor applications. When tested in 1 M H2SO4 electrolyte with cyclic voltammetry analysis, the material delivered rectangular-type CV curves demonstrating the pure EDLC-type behavior. The electrode material delivered 165 F/g of specific capacitance at the current density of 1 A/g. The present work can be further extended to produce redox electrolyte based supercapacitor or the doping of heteroatoms in the gas pyrolyzed carbon structure

ACKNOWLEDGMENTS

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowaska-Curie grant agreement No. 101065296 and 847639.

Composite Materials Based On Thermally Expanded Graphene and Metal Nanostructures In A Polymer Matrix for Solid-State Batteries.

Alena Shumskaya[1*], Alexander Kornev[1], Serhei Kostevich[2]

[1]*R.SC. Real Scientists Cyprus Ltd (Cyprus)*

[2] *ASBISc Enterprises PLC (Cyprus)*

lunka7@mail.ru

Abstract ID #NEE- 853

Solid State Batteries (SSB) is a battery design uses solid film electrodes and solid state electrolytes instead of liquid ones. SSB can solve problems with flammability, limited voltage, electrolyte phase instability, low duty cycles. The problems of SSB are the high interfacial resistance between the cathode and the solid an electrolyte, the low conductivity of the electrolyte. The aim of this work is to develop composite materials based on thermally expanded graphene (TEG) and metal nanostructures in a polymer matrix with high conductivity and the possibility of sequential formation of active layers for solid-state batteries.

The proposed SSB design is a multilayer thin-film elastic structure made of composites of metal nanoparticles and polymer matrix. In this case, the electrode layers are based on an elastic electrically conductive thin film of TEG with agglomerates of anode or cathode metal with size of 50-100 nm deposited on the active side facing the electrolyte, which were obtained by wet chemistry / electrochemical deposition of metal on the TEG film surface. To demonstrate the technology, a copper / zinc pair was chosen, the thin films of which were obtained galvanically. Pairs of metals can be customized to control the following properties: the available potential difference, the amount of active substance, the presence of an oxide phase to form devices for various areas of use of TA. PVA was chosen as the polymer matrix of electrodes and electrolyte, and PMMA was chosen for the separator placed between the electrodes. Both polymers perform the function of binding, with the addition of 10 wt.%. The resistance of such film materials with a thickness of 15 microns and conductivity ranges from 0.5 to 7.3 Ohm. The electrolyte layer consists of an elastic polymer matrix with the inclusion of carbon or silicon nanoparticles to increase conductivity, coated with polyaniline. The NaCl solution is dispersed in the electrolyte structure to allow charge transfer during charging/ discharging cycles. The use of polyaniline is a distinctive feature of the proposed design and allows you to increase the conductivity of the solid state electrolyte. PVA forms an elastic matrix for the electrolyte, in addition, being a hydrogel, increases electrical conductivity.

We have obtained electrode materials for SSB based on TEG, where all layers are composite polymer films, not more than 15 μm thickness, with high conductivity and mechanical stability.

Facile Fabrication of Flexible Zinc Oxide Nanostructured Materials for Applications in Thermoelectric Generators

Raitis Sondors*, Margarita Baitimirova, Donats Erts, Jana Andzane

University of Latvia, Institute of Chemical Physics (Latvia)

raitis.sondors@lu.lv

Abstract ID #NEE- 855

More than half of the energy used to generate electricity is lost as waste heat. High peformance thermoelectric materials can be used to capture the wasted heat. Commercially available high peformance thermoelectric generators usually employ metal chalcogenides, which are expensive due to their scarcity, and are easily oxidized [1], thus altering their electric and thermoelectric properties. In order for thermoelectric generators to be used for a broad range of applications on a wide variety of heated surfaces, cheap, environmentally friendly flexible thermoelectric materials must be developed.

Previous research has shown zinc oxide (ZnO) to possess desirable thermoelectric properties [2], however its low electric conductivity and high thermal conductivity prevents its use in high performance thermoelectric generators. Nanostructuring has been shown to be a viable way to improve the thermoelectric efficiency of ZnO based materials [3]. In our work we have developed methods for fabricating flexible nanostructured ZnO layers on various surfaces for use in thermoelectric generators. By adjusting synthesis parameters we were able to affect the morphology and improve the thermoelectric properties of the resulting material. Our measurements indicate a higher Seebeck coefficient and electrical conductivity than the vast majority of previously published results for ZnO based thermoelectric materials.

Our results show that flexible ZnO nanostructures are a promising material for use in flexible thermoelectric generators. The use of ZnO based thermoelectric materials could facilitate the production of cheap, environmentally friendly flexible thermoelectric generators for a broad range of use cases.

ACKNOWLEDGMENTS

This research was supported by the ERDF, project No. 1.1.1.1/20/A/144 ("Development of nanostructured thermoelectric materials and their application in thermal insulation panels to increase the energy efficiency of buildings"). Project co-financed by REACT-EU to mitigate the effects of the pandemic crisis.

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Beta Vulgaris-Derived Activated Carbon Electrode Coupled With a Redox Additive Electrolyte for Hybrid Supercapacitor

Ashwinder Kaur[1,2*], Vishal Shrivastav[3], Shashank Sundriyal[4], Isha Mudahar[1], Sunita Mishra[5]

[1] *Punjabi University.Patiala India (India)*
[2] *CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C Chandigarh (India)*
[3] *Institute of Physical Chemistry-Polish Academy of Sciences (IChF), Poland (Poland)*
[4] *CATRIN-RCPTM Palacky University Olomouc, Czech Republic (Czech Republic)*
[5] *Academy of Scientific and Innovative Research (India)*

ashsandhu101@gmail.com

Abstract ID #NEE- 858

Supercapacitors (SCs) are thought to be the best option for high-power electrochemical energy storage applications because they are intermediate between conventional capacitors and batteries [1]. Further, redox-enhanced supercapacitors achieve high specific capacitance by adding redox-active additives to the electrolyte, which provide additional faradaic pseudo-capacitance [2]. In this context, biowaste-derived activated carbon is venerated for SC to get higher specific capacitance & cyclic stability. In this work, Beta vulgaris waste (peel & leaves) derived activated carbon (BV-AC) was prepared by carbonization in an acidic medium followed by chemical activation in potassium hydroxide under N2 flow [3]. The structure, morphology & chemical functionalities were confirmed by XRD, FESEM, and FT-IR in prepared porous carbon. The charge storage mechanism of activated carbon has been studied in a neutral aqueous medium (1 M Na2SO4) as well as in a stable couple redox additive electrolyte (0.2 M K3[Fe(CN)6]- 1 M Na2SO4) to optimize a symmetric (or hybrid) supercapacitor. The electrical double layer based on BV-AC/Na2SO4 shows the nearly rectangular CV curve within a potential of 0-1 V. On adding the redox additive to Na2SO4, the K3[Fe(CN)6] gives a large absolute area & additional pair of redox peaks in CV curves (0-1V). Coupling BV-AC with 0.2 M K3[Fe(CN)6]-1 M Na2SO4 enables the operation of a symmetric device at 2.0 V, which is much higher than the thermodynamic decomposition voltage of water. Thus, this is the viable and clear approach to the processing of BV-AC electrodes for next-generation low-cost hybrid supercapacitors.

ACKNOWLEDGMENTS

The authors thank the director CSIR-Central Scientific Instruments Organization (CSIR-CSIO), Chandigarh, India for providing experimental facilities and other infrastructural facilities to perform experimental work. The authors are grateful to the Department of Science & Technology for providing financial support under sanction no. [DST/WOS-A/PM-5/2021].

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Fabrication of Cu_2O Nanowire Networks for Thermoelectric Applications

Davis Gavars[1*], Raitis Sondors[1], Anatolijs Sarakovskis[2], Artis Kons[1], Donats Erts[1], Jana Andzane[1]

[1] *University of Latvia, Institute of Chemical Physics (Latvia)*
[2] *Institute of Solid State Physics, University of Latvia (Latvia)*

davis.gavars@lu.lv

Abstract ID #NEE- 859

Unused emitted heat is a form of energy waste, which lowers the efficiency of any system. Thermoelectric generators (TEGs) can be used to harvest the wasted energy for passive power generation, thus mitigating the loss and increasing the power efficiency. Currently TEGs are mainly used in an industrial capacity and generally consist of materials like Bi2Se3 or Bi2Te3, which are dangerous and expensive [1]. To facilitate the use of TEGs in various settings, more affordable and safer alternative materials, like copper oxides should be used. The fabrication of CuO nanowires from copper foil by thermal oxidation is a well-known method [2], however further annealing of CuO to synthesize Cu2O nanowires has not been previously reported. The current methods for obtaining Cu2O nanowires usually involve various reducing agents reacting with copper (II) salts and strong alkali [3].

Here we show a new method for Cu2O nanowire network fabrication, that can provide a better alternative to the ones currently used. The method is based on CuO nanowire synthesis by thermal oxidation of copper foil and further annealing to produce Cu2O nanowires. The fabricated Cu2O nanowire networks showed a high Seebeck coefficient [4]. Our results show that copper oxide nanowire networks with a high Seebeck coefficient can be efficiently obtained from copper foil and their thermoelectric properties provide many different applications for these materials.

ACKNOWLEDGMENTS

This research was supported by the ERDF, project No. 1.1.1.1/20/A/144 ("Development of nanostructured thermoelectric materials and their application in thermal insulation panels to increase the energy efficiency of buildings"). Project co-financed by REACT-EU to mitigate the effects of the pandemic crisis.

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Finite Element Analysis of Composite Materials Reinforced with Flawed Nano-Particles

Waleed Ahmed*

UAE University (United Arab Emirates)

w.ahmed@uaeu.ac.ae

Abstract ID #NEE- 884

The main objective of this research is to utilize the finite element method as an effective tool for accurately predicting the effective stiffness of a composite material reinforced with nano-particles. The analysis focuses on two specific scenarios. Firstly, it investigates a case where the nano-particles act as ideal reinforcements, assuming they remain completely intact throughout the analysis. Secondly, the study explores a scenario where the nano-particles are assumed to be fully defective or fractured. To conduct the analysis, a linear elastic, finite element approach is employed. The stiffness of the particles plays a critical role in the investigation, as it significantly affects the overall behavior of the composite material. Furthermore, the analysis considers various particle volume fractions to assess their influence on the effective modulus of elasticity for the examined cases. By examining these factors, the study aims to enhance our understanding of the mechanical properties of composite materials reinforced with nano-particles, providing valuable insights for practical applications and design considerations.

Application of MoS_4^{2-} Intercalated Magnetic Layered Double Hydroxide for Preconcentration of Cadmium and Lead From Water Samples

Luthando Nyaba[1,2*], Philiswa Nosizo Nomngongo[1, 2]

[1] *Department of Chemical Sciences, University of Johannesburg, Doornfontein, Johannesburg 2028 (South Africa)*

[2] *Department of Science and Innovation-National Research Foundation South African Research Chairs Initiative (DSI-NRF SARChI) in Nanotechnology for Water, University of Johannesburg, Doornfontein, Johannesburg 2028 (South Africa)*

lnyaba@uj.ac.za

Abstract ID #NEE- 894

A MoS_4^{2-}–intercalated magnetic FeMgAl layered double hydroxide (Fe_3O_4@ MoS_4^{2-}–FeMgAl LDH) nanocomposite was synthesised via hydrothermal assisted exfoliation. The material was applied as the adsorbent for extraction, preconcentration and removal of cadmium ions (Cd^{2+}) and lead ions (Pb^{2+}) from wastewater and river water. The structural properties and morphologies of the adsorbent were determined by transmission electron microscopy, scanning electron microscopy coupled with energy dispersive spectroscopy, Fourier transform infrared spectroscopy, zeta potential and X-ray diffraction. The parameters influencing the preconcentration and adsorptive removal process were optimised using the central composite design (CCD) method. The concentrations of Cd^{2+} and Pb^{2+} in the samples were determined using inductively coupled plasma optical emission spectrometry (ICP-OES). The preconcentration method developed in the study was ultrasound-assisted magnetic solid phase extraction (UA-MSPE). Under optimum conditions, linearity was 0.1-800 µg/L with the correlation of determination (R2) of 0.9987.

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Hybrid CdSe/ZnS Quantum Dots-Gold Nanoparticles Composites Assembled by Click Chemistry for Redox Photocatalysts Applications

Pierre Bauer[1], Aude Barbara[1], Ali Dabbous[2], Vincent Maurel[2], Fabien Dubois[1*]

[1] *Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 25 rue des martyrs, 38000 Grenoble (France)*
[2] *CEA-Grenoble/Inac/Symmes, 17 rue des Martyrs 38054 Grenoble (France)*

fabien.dubois@neel.cnrs.fr

Abstract ID #NEE- 907

At the Neel institute, we work on different approaches to assemble isolated (Au, Ag, quantum dots) nanoparticles to obtain controlled aggregates of different sizes and compositions to develop new correlation spectroscopy methodologies and photocatalysis applications.

In this context, we published different works concerning the spontaneous formation of silver nanoparticles aggregates in the presence of small organic molecules such as mercaptobenzoic acid (MBA) [1, 2] . The trapping of MBA molecules in between the nanoparticles provokes an intense SERS signal due to their presence within the electromagnetic hotspot arising from the association of the spherical particles. In these conditions, we demonstrated that the measurement of the temporal fluctuation of this SERS signal (SERS Correlation Spectroscopy) is enabled to determine quantitatively and in situ the size of the SERS active clusters.

To obtain a more controlled evolving system with a specific spectroscopic signature of the formation of aggregation states, we are currently developing the growth of clusters of particles using the formation of new chemical bonds formed by chemical reactions between functional ligands present on the surface of the starting system. This versatile strategy opens the way to prepare original hybrid materials composed by different types of particles such as semiconducting quantum dots nanoparticles (QDs) covalently fixed to the surface of metallics nanoparticles (hybrid metallic NP-QDs). This project proposed to investigate a new class of photocatalysts based on colloidal quantum dots that are expected to be i/ affordable, ii/ working with visible light and iii/ able to photocatalyze redox reactions in smooth conditions [3] . The originality of the systems developed in this project will be the controlled size connections of quantum dots with metallic nanoparticles. Such aggregates quantum dots/metallic nanoparticles obtained promote the electron/hole separation by electron transfer from the quantum dots to the metallic nanoparticles and improved the efficiency of the photocatalytic systems in water. The composites are characterized by different typical technic concerning nanoparticles suspensions: DLS, FCS, zetametry, SEM imaging, UV-visible spectroscopy, fluorescence spectroscopy. We aimed to improve the photocatalytic activity of CdSe/ZnS core-shell QD in water for 8-oxo-dG oxidation and nitrophenylalanine derivatives reduction, that our group has reported previously [4] . The reaction photocatalyzed by the QD-AuNP composites reached much higher turnover numbers for the conversion of 8-oxo-dG than the QD alone (more than 2600 in 3 hours vs. 350 for QD alone) and appeared to be much faster since a TON of 1500 was observed in 10 minutes.

ACKNOWLEDGMENTS

This work the ANR (projec ANR-18-CE93-0004).

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TRACK 11

“NANOBIOMEDICAL RESEARCH & APPLICATIONS”

Various Strategies for DNA Identification Using Surface Enhanced Raman Scattering

Andrzej Kudelski *

Faculty of Chemistry, University of Warsaw (Poland)

* akudel@chem.uw.edu.pl

Abstract ID #NRA-0471

The deoxyribonucleic acid (DNA) is the carrier of genetic information for all living organisms. Even a small mutation in its structure can lead to the development of a serious disease. Therefore, many scientists are working on developing fast, sensitive and precise methods for detecting specific DNA fragments. One of very promising analytical method used for detecting and identifying of many compounds, including DNA [1-4], is surface-enhanced Raman scattering (SERS). In the SERS effect, for molecules located at or near the surface of nano-plasmonic structures, the efficiency of the generation of Raman signal can be increased by many orders of magnitude. Sometimes, the efficiency of generation of SERS signal is so large, that it is possible to record a good quality SERS spectrum even of a single molecule [5]. Therefore, SERS is one of the most sensitive analytical tools.

In this contribution, we developed a new method of DNA detection using SERS spectroscopy and we compare the method developed with some standard SERS DNA detection methods. The "working" part of the new SERS DNA sensor developed contains capture single-stranded DNA with an attached alkanethiol linking moiety (capture HS-ssDNA) and 6-mercaptohexan-1-ol chemisorbed on the gold or silver SERS substrate. Hybridization with the target ssDNA, complementary to the chains of immobilized capture HS-ssDNA, induces changes in the conformation of the chains of chemisorbed ω-substituted alkanetiols (6-mercaptohexan-1-ol and the alkanethiol linking moiety of HS-ssDNA), which can be easily observed using SERS spectroscopy. Developed new SERS DNA (bio)sensor has been tested on clinical samples and is characterized by the low detection limit at the level of μg/L, wide analytical range from ca. 7 μg/L to ca. 70 mg/L and high selectivity.

We also analysed influence of some parameters on the efficiency of one of the standard SERS DNA sensors, so-called sandwich-type SERS DNA sensor. We tested, for example, attaching a Raman reporter moiety (a chromophore with very large cross section for Raman scattering) at various places of the reporter DNA chain or using various plasmonic materials as SERS substrates. We found that, although in general there is an increase in the intensity of the SERS signal when the distance between the Raman scatterer and the SERS-active surface decreases, for this type of SERS DNA sensor a greater intensity of the measured Raman signal is usually observed when the Raman reporter is farther away from the plasmonic substrate. This is probably caused by a significant change in the hybridisation efficiency for the different structures of the sensor analysed due to some steric hindrances.

We hope that our results will help in the construction of more sensitive and effective SERS DNA sensors and that in the near future, SERS spectroscopy will be a standard method for detecting gene mutations.

ACKNOWLEDGMENTS

This work was financed by the National Science Centre, Poland, project No. 2019/35/B/ST4/02752.

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Interaction of Silver Nanocluster $(Ag)_{26}$ with various Anti-inflammatory Drugs Ciprofloxacin, Levofloxacin and Moxifloxacin

Bijal Rajeshkumar Mehta[1 *], Sutapa Mondal Roy[2], Debesh R. Roy[1]

[1] *Sardar Vallabhbhai National Institute of Technology (India)*

[2] *Sir P. T. Sarvajanik College of Science, Veer Narmad South Gujarat University (India)*

* m.bijalr92@gmail.com

Abstract ID #NRA-0477

We have investigated nano-bio interactions between silver nanoclusters and various anti-inflammatory drug molecules, viz. Ciprofloxacin (Cp), Levofloxacin (Lv) and Moxifloxacin (Mx). We have developed an Ag_{26} nanocluster with dimension 1.2 nm as a model nanoparticle and studied its nano-bio interactions with Cp, Lv, and Mx. The silver nanoparticles (AgNPs) are non-toxic, inert, stable, and have a high binding capacity to the biological environment. AgNPs, due to their effectiveness for plenty of bio-applications, have already been synthesized via environmentally benign routes by our group in the past and have been utilized to demonstrate significantly high biocompatibility, lower cellular toxicity, and higher antibacterial activities in several studies [1, 2]. In the present work, theoretical using density functional theory (DFT) using VASP software on the Ag_{26} and antibiotic drugs (Cp, Lv, and Mx) complexes are investigated to understand the comparative interaction of these drugs with the model nanoparticle and their atomic distances ranges between 1.42 Å to 3.29Å. The optical properties are calculated in which Ag26 and antibiotic drugs (Cp, Lv, and Mx) complexes interaction has UV-Vis range of (λ=320 Åto 953 Å). These drugs are widespread, amply consumed therapeutic to treat bacterial infection. Theoretical investigations have shown that Levofloxacin interacts maximum with model nanoparticles in terms of electron transfer (ΔN) and energy transfer (ΔE), implying the best drug-nanoparticles assembly and can be good antibiotic therapeutics as compared to bare drugs.

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Effect of Clinoptilolite Doped with Cations of d- and f-metals on Viability of Tumor Cells Depends on Density of Intercellular Contacts and Rate of their Growth

Iryna Ivasechko[1 *], Olga Klyuchivska[1], Volodymyr Vasylechko[2], Olga Vyviurska[3], Yaroslav Kalychak[4], Rostyslav Stoika[5]

[1] *Institute of Cell Biology, NAS Ukraine (Ukraine)*
[2] *Ivan Franko National University of Lviv, Lviv University of Trade and Economics (Ukraine)*
[3] *Slovak University of Technology in Bratislava (Slovakia)*
[4] *Ivan Franko National University of Lviv (Ukraine)*
[5] *Institute of Cell Biology, NAN Ukraine (Ukraine)*

* irynagrytsyna@gmail.com

Abstract ID #NRA-0485

Zeolites are biocompatible materials demonstrating an extended application in different areas, including medicine and diagnostics. For enhancement of biological effects of zeolites, their surface may be modified via introduction of reactive chemical groups (carboxy, amino, hydroxy, others), or through doping with cations of d- and f-metals. We used natural zeolite clinoptilolite mined in Transcarpathian region of Western Ukraine. This mineral demonstrates meets most of requirements for multifunctional nanomaterials, and it contains big amount of surface silanol (–OH) groups. Here, we prepared clinoptilolite doped with cations of d- and f-metals, as well as and its H-form, and investigated the effect of these agents on the viability (MTT assay) and morphological characteristics of human tumor cells. We have found differential effect of the prepared agents on intestinal carcinoma cells of HCT-116 line that grow in monolayer culture with tight contacts between cells and relatively low proliferation rate, and the acute T-leukemia cells of Jurkat line that grow in suspension without direct contacts between cells and possessing high proliferation rate. Earlier, we have shown that clinoptilolite dopped with Ag+ possessed antimicrobial activity, was irreversibly adsorbed by malignant cells, and inhibited their viability in vitro. Here, we demonstrated that doping of H-clinoptilolite particles with rear earth cation Tb(III) enhanced their anticancer potential in vitro. H-clinoptilolite-Tb(III) compositions complexed with organic components (1,10-phenanthroline and atophan) demonstrated more intense green and yellow-red luminescence, compared to compositions without such components. The detected peculiarities of luminescence of studied complexes might be defined by different influence of clinoptilolite microcrystals on intercellular contacts of suspension and monolayer cells. The detected effects of the clinoptilolite and its H-form doped with cations of d- and f-metals on viability of tumor cells suggests differential action of these agents towards solid tumors versus leukemias and lymphomas.

ACKNOWLEDGMENTS

State budget topic of the Faculty of Chemistry of of Ivan Franko National University of Lviv XA-32F "New compositions of metal-clinoptilolite for the needs of analytical chemistry, biology and health care" state registration number 0122U001599 (2022-2024)

Freeze-thawing Condition to Obtain the Chitosan-Calcium Phosphate Composites with Controllable Degradation Degree

Liudmyla Sukhodub *, Mariia Kumeda, Leonid Sukhodub, Olexandr Tsyndrenko

Sumy State University (Ukraine)

* l.sukhodub@gmail.com

Abstract ID #NRA-0499

A nerve conductor (conduit) for the treatment of damaged peripheral nerves should not only provide mechanical support for the growth and recovery of the nerve but also minimize its compression during recovery, and the optimal time of its biodegradation should correspond to the recovery period of the damaged nerve [1].

The hybrid material synthesized in this work for potential use as nerve conductors is a chitosan matrix with uniformly distributed calcium phosphate particles. The applied multistage synthesis includes a repeated process of two processes. The first one is freezing of the colloidal suspension of precursors containing chitosan and calcium acetate at a temperature of -18°C. The second process is afterwards thawing: a) at room temperature, b) under the influence of microwave irradiation. All samples cross-linked in a sodium phosphate solution at a temperature of 4°C gradient thawing. This caused in situ formation of microparticles of nanocrystalline amorphous calcium phosphate (ACP) and brushite (DCPD).

Degradation of the synthesized biomaterial in vitro was studied in SBF solution [2], which is similar in composition to the physiological fluid of the human body. The results prove that the degradation of single-time frozen sample 1 is the smallest. It begins after 15 days of immersing in SBF and occurs at a rate of 0.4% per day. At the same time, the degradation of samples 2 and 3 begins after one day at a rate of 0.95 and 0.75% per day, respectively.

According to the XRD data, it was determined that in the samples annealed at 900 oC, the share of monetite formed during the thermal transformation of brushite increases in the following order: 1 < 2 < 3. It is evident that during degradation, the dissolution of this particular calcium phosphate compound occurs first, which affects the time of the material's complete degradation. It should be noted that the time of biodegradation of all samples corresponds to the healing period of the damaged nerve.

Thus, by adjusting the type of freeze-thawing during the synthesis of hydrogel based on chitosan and calcium phosphate, it is possible to influence the time of its degradation.

ACKNOWLEDGMENTS

The research was financially supported by the Ministry of Science of Ukraine in the frame of a research topic 0122U000775.

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RE^{3+}-doped Ceria Nanoparticles with Spectroscopically Controlled ROS Scavenging Activity

Vladyslav Seminko *, Pavel Maksimchuk, Vladimir Klochkov, Yevhen Neuhodov, Svetlana Yefimova

Institute for Scintillation Materials, NAS of Ukraine (Ukraine)

* seminko@ukr.net

Abstract ID #NRA-0501

Ceria (CeO_{2-x}) and ceria-based nanoparticles nowadays are well-known due to their unique enzyme-like catalytic activity making these materials indispensable for a number of biomedical applications [1]. These nanoparticles are more robust, more stable under extreme pH and temperature conditions and also much cheaper than natural enzymes. At the same time, as the mechanisms of anti-/prooxidant action of these nanoparticles, so the ways to control their redox activity during interaction with ROS (reactive oxygen species) are discussed in a number of publications [2, 3].

We have obtained and studied luminescence and antioxidant properties of RE^{3+} (RE = Y, Tb, Eu)-doped colloidal ceria nanoparticles. The luminescence of nanoceria was excited by a continuous-wave GKL-4UM He-Cd laser (~325 nm) and registered using the SDL-1 grating monochromator with the Hamamatsu R9110 PMT in the photon counting mode.The processes of hydrogen peroxide (HP) decomposition by ceria nanoparticles were studied using the change of the characteristic HP absorption band (200-250 nm) recorded using Specord 200 spectrophotometer (Analytik Jena, Germany). Immediately after hydrogen peroxide addition to aqueous colloidal solutions of nanoceria the time evolution of Ce^{3+} luminescence intensity (taken at 425-430 nm) was determined by means of time-resolved measurements. We have shown that luminescence endowed by RE^{3+} doping of ceria nanoparticles as well as Ce^{3+} luminescence can be used for tracing of the processes of ROS-nanoceria interaction using the methods of conventional optical spectroscopy. The quenching effect of hydroxyl groups formed on the surface of ceria NPs during decomposition of hydrogen peroxide leads to reversible change of RE^{3+} luminescence intensity. Monitoring this intensity provides information on both the dynamics and the mechanisms of ROS scavenging by nanoceria. At the same time, we have seen the sufficient slowdown of $Ce^{4+} \rightarrow Ce^{3+}$ recovery process and decrease of HP decomposition rate for RE^{3+}-doped nanoceria as compared to undoped ceria NPs.

Generally, the ceria-based NPs as a new type of redox-active nanoparticles with ability both to scavenge/produce reactive oxygen species and to visualize the change in ROS concentration during this process are promising for a number of applications, while controlling the processes of recovery of undoped and doped nanoceria HP luminescence sensors provides an additional advance over traditional sensors based on organic molecules or enzymes. These luminescent sensors are reversible and their recovery rates can be sufficiently increased by temperature and continuous UV irradiation. At the same time, high concentrations of RE^{3+} ions can deteriorate the catalase-mimetic activity of ceria nanoparticles and worsen their antioxidant properties that should be keep in mind while using these sensors in biological media.

ACKNOWLEDGMENTS

This research was supported by National Research Foundation of Ukraine for Leading and Young Scientists Research Support, Grant No. 2020.02/0052

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Silver Nanotriangles Incorporated Gum Tragacanth/ Sodium Alginate Hydrogels for Biofilm Inhibition

Deepa Garg[1 *], Abhay Sachdev[1], Ishita Matai[2]

[1] *Central Scientific Instruments Organisation, Chandigarh, India (India)*
[2] *Amity University, Punjab (India)*

* deepagarg170@gmail.com

Abstract ID #NRA-0505

Implant infections arising from microbial colonization and biofilm formation impair the tissue integration process [1]. Present-day preventive and treatment approaches are highly dependent on conventional antibiotic therapies but the rise in antibiotic resistance is a major limitation [2]. This created a need for developing non-antibiotic antimicrobial agents to avoid the fear of developing resistance. In this regard, triangular silver nanoparticles (AgNTs) with broad-spectrum antibacterial potential have been explored for antibacterial applications [3]. Furthermore, there is a growing consensus that natural polymer based hydrogel coatings on implants can prevent microbial adhesion with localized release of antimicrobial agents [4]. Nevertheless, the problem of complicated hydrogel synthesis persist. We aim to propose a simple process for natural polymer based hydrogel coatings that could prevent microbial adhesion at low concentrations of AgNTs. On that account, we developed hydrogels using composite bactericidal hydrogels were fabricated by incorporating AgNTs into a hybrid polymer network of Gum Tragacanth/Sodium Alginate (GT/SA). Notably, the hydrogels were formed rapidly within 15 minutes. The rheological studies showed that the mentioned hydrogels possess good stability and mechanical strength, with storage modulus in the range of 400-900 Pa. The antibacterial effectiveness of the AgNT-hydrogel was tested against both planktonic and biofilm-forming Gram-negative (*Escherichia coli* and *Pseudomonas aeruginosa*) and Gram-positive (*Staphylococcus aureus*) bacteria. The AgNT-hydrogel exhibited a dose-dependent decrease in bacterial growth for all strains, inhibiting 87 % of planktonic biomass and reducing biofilm formation by up to 74 % when added at concentrations of 40-80 mg ml^{-1}. Overall, our findings suggest that the synthesized hydrogels can significantly prevent local bacterial infections related to implants.

ACKNOWLEDGMENTS

Authors would like to thank CSIR-CSIO, Chandigarh for providing access to the various analytical facilities. Sincere thanks to Science and Engineering Research Board (ECR/2018/000199/ES), and Council of Scientific & Industrial Research (MLP 2006), India for providing the support and financial assistance for this work. The author is thankful to the Department of Biotechnology, Government of India, for the fellowship.

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Oxide Nanocrystals with Variable Valence Ions for Hydroxyl Radical Neutralization

Pavel Maksimchuk[1 *], Kateryna Hubenko[1, 2], Yevhen Neuhodov[1], Vladyslav Seminko[1], Andrey Onishchenko[3], Iryna Bespalova[1], Vladimir Klochkov[1], Lesya Demchenko[4, 5], Svetlana Yefimova[1]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *Leibniz Institute for Solid State and Materials Research Dresden (IFW) (Germany)*
[3] *Kharkiv National University of Radio Electronics (Ukraine)*
[4] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
[5] *Stockholm University, Department of Materials and Environmental Chemistry (Sweden)*
* pavel.maksimchuk@gmail.com

Abstract ID #NRA-0508

The process of cellular respiration in living cells leads to the formation of biologically active molecules called reactive oxygen species (ROS) [1]. These ROS, namely superoxide anions, hydrogen peroxide, and hydroxyl radicals, are produced inside the mitochondria and play indispensable role in the metabolism of the cell [2]. At the same time, an increase of the content of hydroxyl radicals (·OH) which are the strongest oxidants among all reactive oxygen species can trigger the number of pathological processes inside the cell from enhanced lipid peroxidation of cell membranes to DNA damage [3].

Hydroxyl radicals are formed at water radiolysis during X-ray or gamma-irradiation of the cell [4]. Extremely high reactivity of these radicals, with an average lifespan of only a few nanoseconds in a biological environment, makes it quite challenging for the cell's internal systems to effectively neutralize them. We propose three different types of oxide nanocrystals with variable valence ions (CeO_2, TiO_2 and $GdVO_4$) as promising materials for effective neutralization of hydroxyl radicals.

Synthesized CeO_2, TiO_2 and $GdVO_4$ nanocrystals were characterized using transmission electron microscopy, X-ray diffraction and X-ray photoelectron spectroscopy. For detection of the hydroxyl radical neutralization in aqueous solutions luminescence spectroscopy and specific probe coumarin was used. The detection of hydroxyl radicals in the solution is accomplished by observing the formation of a fluorescent product, 7-hydroxycoumarin, resulting from the oxidation of coumarin by hydroxyl radicals. This product appears as a new fluorescent band with a peak at 460 nm.

CeO_2, TiO_2 and $GdVO_4$ nanocrystals exhibit remarkable ROS neutralizing capabilities against hydroxyl radicals generated in water solutions during X-ray irradiation. Hydroxyl radicals scavenging properties of nanocrystals have been found to be closely linked to the high amount of reduced variable valence ions (such as Ce^{3+} in CeO_2, Ti^{3+} in TiO_2, V^{4+} and V^{3+} in $GdVO_4$), which have the ability to donate electrons in hydroxyl radical neutralization reaction. Small oxide nanocrystals are characterized by the presence of high content of structural imperfections, such as oxygen vacancies. The reduction of neighboring variable valence ions can occur with the formation of oxygen vacancies, as confirmed by XPS experiments for all three different types of oxide nanocrystals (CeO_2, TiO_2 and $GdVO_4$). The capability of small oxide nanocrystals containing variable valence ions (CeO_2, TiO_2 and $GdVO_4$) to efficiently neutralize hydroxyl radicals in aqueous solutions suggests their potential as effective antioxidants and radioprotectors in living cells.

ACKNOWLEDGMENTS

Acknowledgments: This research was supported by National Research Foundation of Ukraine, Grant № 2020.02/0052 for Leading and Young Scientists Research Support.

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Catalytic Effect of $GdVO_4:Eu^{3+}$ Nanocrystals Over H_2O_2 Decomposition Reaction

Svetlana Yefimova[1 *], Pavel Maksimchuk[1], Kateryna Hubenko[1, 2], Vladimir Klochkov[1], Oleksandr Sorokin[1], Vladyslav Seminko[1], Lesya Demchenko[3, 4]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *Leibniz Institute for Solid State and Materials Research Dresden (IFW) (Germany)*
[3] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" (Ukraine)*
[4] *Stockholm University, Department of Materials and Environmental Chemistry (Sweden)*
* ephimovasveta@gmail.com

Abstract ID #NRA-0509

Recently, nanoparticles with intrinsic antioxidant properties have attracted a great deal of interest as an inorganic alternative to conventional organic antioxidants [1]. It is generally accepted that the imbalance between reactive oxygen species (ROS) production and scavenging at a cell level causes the development of oxidative stress that overwhelms the antioxidant capacity of cells and leads to the accumulation of irreversible damage to proteins, lipids, and DNA, as well as the development of numerous pathologies, including neurogenerative diseases, cancer, cardiovascular diseases etc. Hydrogen peroxide (H2O2) is one of ROS molecules involved in most of the redox metabolism reactions and processes of the cells. H2O2 is considered to play a central role in a cell's homeostatic metabolism as a mediator of several physiological processes, such as cell differentiation and proliferation, survival, and immune response [2]. At the same time, the main source of initiation of biomolecules oxidation reaction is the Fenton reaction between H2O2 and Fe2+ ions with highly reactive hydroxyl radicals (•OH) production. Thus, antioxidants that react with H2O2 without generation free radicals, such as •OH, are of special interest as preventive antioxidants.

In the present work, we analyze the mechanism of H2O2 decomposition by GdVO4:Eu3+ nanocrystals (NCs) in a water solution using the optical spectroscopy technique. TEM imaging reveals that synthesized GdVO4:Eu3+ nanoparticles possess crystal structure and an ellipsoid-like form with l=12.1±1.23 nm and d=5.76±0.68 nm. XPS analysis showed that vanadium ions in the crystal lattice could be found in the V5+ (44%), V4+ (43%), and V3+ (13%) oxidation states that point to the electron donating properties of GdVO4:Eu3+ NCs and radical scavenging ability. We analyze the possibility of Fenton- and catalase-like reactions in the system. However, we did not detect a Fenton-like reaction with the participation of V4+/V3+ ions and •OH generation. At the same time, it has been revealed that in the system, H2O2 acts as a reductant donating electron to V5+ ions in GdVO4:Eu3+ NCs that was confirmed by increasing the amount of V4+ (56%) and V3+ (30%) ions and decreasing V5+ ions content (14%) and a transformation in the GdVO4:Eu3+ absorption spectrum, as well. Thus, GdVO4:Eu3+ NCs could be prospective as an effective preventive antioxidant for H2O2 decomposition by the catalase-like reaction.

ACKNOWLEDGMENTS

This research was supported by National Research Foundation of Ukraine for Leading and Young Scientists Research Support, Grant No. 2020.02/0052. The authors thank the Armed Forces of Ukraine for the opportunity to continue their research work.

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Surface Characterisation and Anti biofouling properties of Polydopamine based Zwitterion Nano-coatings on Titanium

Supriya Nambiar[1 *], Dilip G Naik[1], Arun M Isloor[2], Ethel Suman[1]

[1] *Manipal Academy of Higher Education (India)*
[2] *NITK, Suratkal (India)*

* supriya.nambiar@manipal.edu

Abstract ID #NRA-0519

In the oral cavity with a multi species bio film environment, clinical infections caused by biofilms are a more challenging healthcare issue, and microbial infections caused by bacterial biofilms on biomedical surfaces are a leading cause of death worldwide. As a result, there is an urgent clinical need to develop coatings for titanium which has better surface characteristics, anti-bacterial effect and improved bio activity in the oral and systemic environment. This study will try to formulate a method for In-house synthesis of Polydopamine zwitterion nanoparticles coatings for titanium. The surface characteristics and antimicrobial properties of the newly synthesized nanomaterial used to coat the titanium surfaces will be analyzed.

To synthesise and optimize the formulation parameters of Zwitterion nanoparticle coatings on Titanium with regard to its physical and anti microbial properties .

10 titanium discs was coated with Polydopamine base which formed a binder and 5 among them was further coated with Zwitterion nanoparticles. The Zwitter nanoparticle characterisation was done to assess particle size and zeta potential. Surface microstructure analysis was done with surface profilometer. Mean surface roughness and quadratic average roughness was calculated.Wettability was measured using a contact angle goniometer automated with image analysis software. Scanning electron microscopy was used to examine the surface characteristics of the modified titanium discs. 5 discs each of the 2 groups (PDA, Zwitter ion + PDA) were studied for Antimicrobial effect using Streptococcus mutans . Each disc was place in the well of a tissue culture plate. 1 ml BHI broth containing Streptococcus mutans grown for 24h and adjusted to 1.5* 10^{8} cfu/ml, was added and the plate was incubated at 370 for 24h. Following this the discs were rinsed twice in Sterile PBS(PH- 7.4). The discs were then vortexed in 1ml PBS to detach the bacteria and then the colony count was done on BHI Agar using in 1: 10,1:100 and 1:1000 dilutions. The colony count were as follows ; PDA – 1.4*10^{5} CFU/ML and Zwitter ion - 1.25*10^{4} CFU/ml.

The Zwitter ion nano coatings were found to be far superior in physical surface characterisation and in biological properties compared to the polydopamine base.

ACKNOWLEDGMENTS

This was carried out at Dr Arun M. Isloor's research laboratory, Dept. of Chemistry, NITK Surathkal-Mangalore,India

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Titanium Oxide Nanoparticles as an Antioxidant for Cryopreservation

Iryna Bespalova[1 *], Mariia Yukhta[2], Viktor Kireev[1], Pavel Maksimchuk[1], Vladyslav Seminko[1], Svetlana Yefimova[1]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *Institute for Problems of Cryobiology and Cryomedicine of the NAS of Ukraine (Ukraine)*
* iiganinabespalova@gmail.com

Abstract ID #NRA-0525

Titanium oxide (TiO_2) nanoparticles (NPs) are well-known due to their excellent photocatalytic properties and manufactured worldwide for a variety of engineering and bioengineering [1]. Recent advances in TiO_2-related photocatalysis are associated with highly defective TiO_{2-x} NPs. It was shown that high amounts of oxygen vacancies, various defects such as Ti^{3+} ions can modifies sufficiently the regular TiO_2 structure and enhance the photocatalytic performance [2]. At the same time, some authors reported on antioxidant properties (ROS scavenging ability) of TiO_{2-x} surfaces and NPs assuming the key role of Ti^{3+}/Ti^{4+} ratio in the TiO_{2-x} structure [2, 3]. Based on these works, we have supposed that TiO_{2-x} NPs could also be successfully used in cryopreservation considering that freezing-thawing process is accompanied by excessive production of peroxide radicals.

In this research, the original method of TiO_{2-x} NPs synthesis based on hydrolysis of titanium butoxide followed by a peptization process has been described. Changing the amount of nitric acid as a catalyst and peptizing agent two types of TiO_{2-x} NPs of the same size about 5 nm, but different $Ti^{3+}(Ti^{2+})/Ti^{4+}$ ratio have been obtained in the form of water colloid solutions, that influences on antioxidant activity NPs. The structure and properties of the obtained TiO_{2-x} NP samples have been analyzed by TEM, XRD, XPS and optical spectroscopy methods. A cytotoxic study also confirmed a good biocompatibility of both obtained samples of TiO_{2-x} NPs. It was shown that in concentration up to 100 mg/L TiO_{2-x} NPs do not affect NIH 3T3 cell morphology as well as their metabolic and proliferation activity during 96-hour cultivation. At the concentration of 200 mg/L TiO_{2-x} NPs with a reduced content of Ti^{2+} ions showed a slight decrease in proliferative activity that was restored when NPs were removed from the culture medium.

The efficiency of TiO_{2-x} NPs during cryopreservation was evaluated after slow freezing of NIH 3T3 cell suspension using trypan blue exclusion tests, propidium iodide staining, alamar blue assay and by cell proliferative activity. The control group was the cells cryopreserved with 5% dimethyl sulfoxide without NPs addition. The results showed that 10 mg/L TiO_{2-x} NPs showed more pronounced effect than another well-known antioxidant CeO_2 NPs (2-3 nm) in the same concentration by all studied parameters.

In conclusion, the application of TiO_{2-x} NPs can be successfully extended on the area of cryopreservation to enhance post thawing cell viability.

ACKNOWLEDGMENTS

This research was supported by National Research Foundation of Ukraine, Grant № 2020.02/0052 for Leading and Young Scientists Research Support.

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Trace Elements as a Specific Marker for Ovarian Cancer Biomineralization

Ruslana Chyzhma[1 *], Roman Moskalenko[2, 1]

[1] *Sumy State University (Ukraine)*
[2] *Ukrainian-Swedish Research Center SUMEYA, Medical Institute, Sumy State University, Sumy (Ukraine)*
* r.chyzhma97@gmail.com

Abstract ID #NRA-0552

Ovarian cancer is the most prevalent cancer of the female reproductive system [1], with epithelial ovarian cancer accounting for 90% of all ovarian malignancies [2]. Unfortunately, specific symptoms are absent in the early stages of the disease [3], and no effective screening strategy is available [4]. As a result, ovarian carcinomas are often diagnosed at the metastatic stage in over three-quarters of patients. Calcification is a significant clinical and morphological indication of ovarian serous adenocarcinoma, which begins in the early carcinogenesis stages [5]. Depending on their size and structure, these calcifications can be visualized using various diagnostic instruments, including ultrasound, CT, and MRI [6].

We studied 30 ovarian cancer samples with (group I) and without (group II) biomineralization. All samples were examined by histology, immunohistochemistry, electron microscopy, atomic absorption spectroscopy, and X-ray diffraction. Here we show the microelement composition difference between groups I and II. We established that zinc (Zn) was decreased in the first group relative to the second by 41.83%. The magnesium (Mg) in the first group was reduced by 52.17%. Iron (Fe) and copper (Cu) in the first group were higher compared to the second group by 91.77% and 7.8%, respectively.

Scanning electron microscopy (SEM) with EDX showed that the main lines of the elemental composition were Ca and P. Their ratio corresponds to the features of hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$.

The immunohistochemical study detected the accumulation of osteopontin (OPN) at the edges of minerals and between lamellae. The difference in OPN expression in the groups of ovarian cancer samples with the presence (73.34 ± 4.25 cells per $1mm^2$) and absence of calcification (26.93 ± 1.88 cells per $1mm^2$, $p<0.001$) indicated their role in biomineralization processes. Fluorescence microscopy showed that OPN-accumulating cells were CD68 positive. It means their direct role in biomineralization processes.

Therefore, considering the elemental composition, it was established that each calcification has structural features that can be used to diagnose and treat ovarian cancer. We demonstrated that macrophages take an active part in the formation of biominerals through the synthesis of osteopontin.

Studying the relationship between the microelement and protein composition of biomineral deposits may be promising for practical application in medical purposes.

ACKNOWLEDGMENTS

This research has been performed with the financial support of grants of the Ministry of Education and Science of Ukraine № 0112U100471 "Condition of mineralized tissues using new composites with Ag+ and Cu2+ nanoparticles.

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Kinetic Biopharmaceutical Studies of a New Paracetamol – Glucosamine Analgetic Drug

Olga V. Vashchenko[1 *], Olena Ruban[2], Igor Zupanets[3], Pavlo Vashchenko[4, 4]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *National University of Pharmacy (Ukraine)*
[3] *JSC Farmak (Ukraine)*
[4] *SSI "Institute for Single Crystals of NAS of Ukraine" (Ukraine)*
* olga_v@isma.kharkov.ua

Abstract ID #NRA-0553

Paracetamol is a worldwide analgesic that is the first-line drug for the treatment of pain and fever in patients of all ages. However, the side effect of paracetamol is hepatotoxicity. N-acetyl-D-glucosamine has a hepatoprotective effect, and their combination leads to increased safety and potentiation of the analgesic effect, which was established by previous studies [1]. Covering paracetamol with a gelatin shell is due to the improvement of its organoleptic properties for the creation of orally disintegrating tablets.

The interaction of drugs with the lipid bilayer of biomembranes is inevitable, since the place of drug administration, their penetration into the systemic bloodstream, entry into the target cell, metabolism, etc. is accompanied by interaction with a large number of cells. It is known that the penetration of most active pharmaceutical ingredients (API) into the cell is carried out by passive diffusion through the lipid bilayer of cells. The interaction of API with the lipid membrane is a mutual process: on the one hand, it affects the pharmacokinetic properties of pharmaceuticals, and on the other, it affects the structural and functional properties of the membranes themselves [1].

Our earlier works demonstrated effectiveness of model lipid membranes application to exploring drugs combinations, especially in kinetic regime [2]. In the present study, multilamellar model lipid membrane of 70 % hydrated *L*-α-dimyristoylphosphatidylcholine (DMPC) was used as testing medium. DMPC membrane undergoes 1st order phase transition 'gel to liquid crystal', or membrane melting, under room temperatures (ab. 25 ºC) which make it convenient to explore drug-membrane interactions without a risk of drug thermal destruction. Phase transition processes were monitored by means of differential scanning calorimetry technique (DSC) using a microcalorimeter Mettler DSC 1 (Mettler-Toledo). DSC profiles were obtained on heating in diapason 0 to 35 ºC. Grounding on the original DSC data, a set of thermodynamical parameters were determined and plotted as functions of time. The mean time of the systems equilibration was ab. 150 hrs.

It was established that gelatin decreased the characteristic time of paracetamol diffusion (τ) about threefold, but it had no pronounced effect on the equilibrium paracetamol penetration into the membrane (D_{eq}). Sole glucosamine manifested no membranotropic effect under the experimental conditions, however, in combination with gelatin, it sufficiently reduced Deq while τ remained within the experimental error. The full drug formulation increased D_{eq} by 30 % in compared with sole paracetamol.

Thus, it can be concluded that some compounds, such as glucosamine and gelatin, can affect both kinetic and equilibrium parameters of paracetamol-membrane interactions, while the developed drug formulation is able to improve paracetamol distribution into DMPC membrane.

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Microstructure of Antioxidants Based on Orthovanadate Nanocrystals: XPS Study

Kateryna Hubenko[1, 2 *], Pavel Maksimchuk[1], Andrey Onishchenko[3], Pavel Potapov[2], Vladimir Klochkov[1], Svetlana Yefimova[1], Martin Knupfer[2]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *Leibniz Institute for Solid State and Materials Research Dresden (IFW) (Germany)*
[3] *Kharkiv National University of Radio Electronics (Ukraine)*

* k.hubenko@gmail.com

Abstract ID #NRA-0559

Oxidative stress (OxS) is a state developed as a result of reactive oxygen species (ROS) overproduction in cells and an ineffective action of cell's antioxidant defense system [1]. It is widely accepted that such factors as stresses, adverse environmental factors and hypercaloric diet cause the overproduction of ROS (hydroxyl radicals, hydrogen peroxide and superoxide anions), which are highly toxic for organism. Overproduction of ROS initiates the irreversible cells damages and can provoke further cell mutations and death [2]. Moreover, OxS is considered to contribute to a variety of diseases, such as diabetes, atherosclerosis, hypertension mellitus, some pulmonary diseases, asthma and cancer [1,2].

Recently, various nanomaterials have attracted growing interest as nano-antioxidants [3]. The antioxidant behavior was shown for such nanomaterials as carbon nanotubes, fullerenes, metal nanoparticles (NPs), metal oxide NPs and various types of antioxidant-loaded polymer NPs [4]. Some oxide NPs were reported to scavenge ROS due to their intrinsic antioxidant mimic properties [5].

In this work we proposed three types of oxide NPs with variable valence ions with different sizes and shapes (extra-small $GdYVO_4:Eu^{3+}$ spheres, small $GdVO_4:Eu^{3+}$ spindles and $LaVO_4:Eu^{3+}$ rods). In order to demonstrate pronounced antioxidant properties, crystal structure of nanoparticle should contain a large number of ions with variable valence in the reduced state (V4+, V3+ and V2+ for vanadium ion), which can donate electron and neutralize ROS or other free radicals. The use of the XPS method made it possible to establish the features of the crystal microstructure of the synthesized nanocrystals, namely, the valence of vanadium ions. XPS studies have shown that a decrease in nanocrystals size leads to an increase of the reduced vanadium ion content. For extra-small $GdYVO_4:Eu^{3+}$ nanocrystals, the number of reduced vanadium ions of oxidation states not characteristic for bulk crystals is more than 60%.

Due to the presence of reduced vanadium ions in the crystal lattice, all three types of nanocrystals are promising for use as antioxidants. The highest concentration of V4+, V3+ and V2+ ions makes extra-small $GdYVO_4:Eu^{3+}$ nanocrystals the most promising for the neutralization of ROS.

ACKNOWLEDGMENTS

This research was supported by the Philipp Schwartz-Initiative of the Alexander von Humboldt-Stiftung.

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Synthesis, Physicochemical Characterization, and Antioxidant Assessment of Biocompatible β-cyclodextrin - Stabilized CeO_2 Nanoparticles

Ganna Grygorova[1 *], Vladyslav Seminko[1], Olga V. Vashchenko[1], Dmitry Sofronov[2], Svetlana Yefimova[1]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *SSI "Institute for Single Crystals of NAS of Ukraine" (Ukraine)*
* grigorova.anne@gmail.com

Abstract ID #NRA-0569

Cerium oxide nanoparticles (nanoceria) are potent free-radical scavengers because of their unique antioxidant properties determined by switching of oxidation states between Ce^{3+} and Ce^{4+} in ambient conditions. The unique redox properties of nanoceria have led to extensive biomedical applications of nanoceria for the treatment of various deceases. Currently, besides antioxidant activity, a pronounced antibacterial, anticancer, anti-diabetic, and tissue regeneration activity of nanoceria was described [1]. Well-studied superoxide dismutase (SOD)-like and catalase-like biological activities provide nanoceria by an ability to eliminate reactive oxygen species (ROS) imbalance in living cells increasing thereby the lifespan of the cells. To increase the antioxidant activity of CeO_2, a variety of methods have been proposed, such as coating nanoceria with organics, doping nanoceria with metal ions, changing the buffer anion, adjusting the size and shape of nanoceria, and so on.

In this work, β-cyclodextrin - stabilized CeO_2 nanoparticles (β-CD@CeO_2) are synthesized by a facile wet chemical route. Cyclodextrins, such as β-CD, have found a vast application for inclusion of water-insoluble molecules and drugs into large (0.66 nm) hydrophobic cavity making them perspective for drug delivery [2]. The β-CD@CeO_2 nanoparticles were characterized by using dynamic light scattering (DLS), transmission electron microscopy (TEM), which revealed the formation of spherical particles in the size range of 2–7 nm. Further analysis by Fourier-transform infrared spectroscopy (FT-IR) does not show covalent bonding between cyclodextrins and CeO_2 nanoparticles suggesting that β-CD is only physically adsorbed on the nanoparticle surface, presumably through hydrophobic interactions which limit the mutual aggregation of nanoparticles. Comparison of β-CD@CeO_2 nanoparticles with citrate-stabilized NPs has shown that presence of β-CD has no deteriorating effect on the antioxidant activity of nanoceria making these materials potent both as antioxidant agents and carriers of water-insoluble antioxidant molecules for obtaining of hybrid nanomaterials with improved antioxidant action.

ACKNOWLEDGMENTS

This research was supported by National Research Foundation of Ukraine, Grant №2020.02/0052 for Leading and Young Scientists Research Support

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Exposure of the Prooxidant Potential of CeO_2 and $GdYVO_4/Eu^{3+}$ Nanoparticles in Model Systems Containing Low-Molecular Antioxidants

Vladimir Klochkov[1], Yuri Nikitchenko[1], Olga Sedyh[1], Yurii Kot[2], Nina Karpenko[1], Galyna Dudetskaya[1], Nataliya Kavok[1 *]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *V. N. Karazin Kharkiv National University, Ministry of Education and Science of Ukraine, Kharkiv, Ukraine (Ukraine)*

* yakavok@gmail.com

Abstract ID #NRA-0574

Nanotechnology-based pro-oxidant strategy for cancer therapy is being actively explored. Attention is drawn to the pro-oxidant properties of nanocerium under certain conditions, as well as its antitumor effect. Thus, the aim of the study—to compare the prooxidant potential of CeO_2 and $GdYVO_4/Eu^{3+}$ NPs as a promoter of ROS-mediated antitumor activity.

2 nm CeO_2 NPs or 2 nm $GdYVO_4/Eu^{3+}$ NPs were used. The oxidative damage to ascorbic acid (AA), NADPH or GSH was monitored by spectroscopic methods at pH 6.7; 7.4; 7.8. The solutions of NPs (with final concentrations of 10-20-40 μg/mL) were added to organic (20 mM Tris or Hepes) buffers contained 200 μmol AA or 200 μmol NADPH or 50 μmol GSH. The mixture was kept for 60 min or 3 h, or 24 h at 37 °C, respectively. The AA oxidative damage was quantified by measuring its absorbance at the characteristic wavelength λ max = 265 nm, NADPH — λ max = 340 nm, and GSH (after reaction with Elman reagent) — λ max = 412 nm using a Specord 200 spectrophotometer (Analytik Jena, Germany).

The literature reports on the potential antitumor activity of rare earth elements (REE) and REE-based nanoparticles, and in particular, much attention is paid to CeO_2 and its combinations with antitumor agents. Data on the antitumor activity of $GdYVO_4/Eu^{3+}$ nanoparticles were also obtained. In the mechanisms of action of nanoceria, the prooxidant potential and, in particular, the ability, under certain conditions, to exhibit oxidase activity with the oxidation of organic substrates is discussed. We have carried out a comparative analysis of the oxidation of the most important low-molecular components of the antioxidant defense system in cells — AA, NADPH, and GSH in the presence of CeO_2 and $GdYVO_4/Eu^{3+}$ NPs. Oxidation of all studied compounds in the presence of CeO_2 NPs was shown. A drop in the level of AA compared with the control was noticed at all studied concentrations of nanoparticles and pH values. At the same time, CeO_2 NPs accelerated the oxidation of NADPH and glutathione only at neutral pH values. Unlike CeO_2, $GdYVO_4/Eu^{3+}$ NPs decrease only GSH and only under weakly alkaline conditions, starting from the lowest NPs concentration (10 μg/mL). It was noted that the oxidation of GSH at pH 7.8 is accompanied by irreversible agglomeration of nanoparticles under these conditions.

Under certain conditions, extra-small CeO_2 NPs demonstrate a significant prooxidant activity, which can damage the antioxidant defense systems of tumor cells that is perspective for the development of NPs-based drugs with antitumor activity.

ACKNOWLEDGMENTS

This work was supported by National Academy of Sciences of Ukraine (Project № 0122U002636)

Dynamics of the Interaction of Rare-Earth-Based Nanoparticles with Glutathione at Physiological pH

Nataliya Kavok[1], Vladimir Klochkov[1], Olga Sedyh[1], Lesia Piliai[2], Galyna Dudetskaya[1 *]

[1] *Institute for Scintillation Materials, NAS of Ukraine (Ukraine)*
[2] *Department of Surface and Plasma Science, Faculty of Mathematics and Physics, Charles University (Czech Republic)*

* gdudetska@gmail.com

Abstract ID #NRA-0580

To assess the effect of pH on the interaction of CeO_2 and $LnVO_4:Eu^{3+}$ (Ln = La, Gd, Y) NPs with low molecular antioxidants (eg, glutathione) in oxidized and reduced forms.

Dynamic light scattering was used to measure the colloidal stability parameters of $GdYVO_4/Eu^{3+}$ (2 nm), CeO_2 (2 nm and 10 nm), $GdVO_4/Eu^{3+}$ (8 × 25 nm), $LaVO_4/Eu^{3+}$ (8 × 80 nm) nanoparticles in the presence of glutathione in aqueous and buffer solutions in the physiological pH 6.7-7.8 range. The hydrodynamic diameter and zeta potential were measured using a ZetaPALS/BI-MAS analyzer (Brookhaven Instruments Corp., USA) operated in the phase analysis light scattering mode. Measurements were carried out at the scattering angle of 90° and λ = 659 nm at t = 25 °C. Zeta potential was negative. The NPs solutions (with final concentrations of 250-500 μg/mL) were mixed in 10 mM HEPES buffer (pH 6.7; pH 7.4 or pH 7.8), the sample also contained GSH or GSSG (2-6 mmol), and 0.2% BSA.

It has been revealed that both forms of glutathione interact with NPs in aqueous and buffer solutions leading to an increase in the hydrodynamic diameter and agglomeration, with the most pronounced changes occurring at the initial stage of the process by the 30th minute of the experiment. Stabilization of solutions due to diffusion was observed during 24-hour incubation. For nanoceria (10 nm) no enlargement in any of the studied systems was observed. Compared to extra-small nanoceria, for orthovanadate NPs of all types, the process was more pronounced, did not depend on the form of glutathione used, and was irreversible under weakly alkaline conditions. Such changes in the aggregation stability of orthovanadate NPs in the presence of glutathione were accompanied by a recharging of the zeta potential, in contrast to nanoceria of both types, for which the potential changes remained negative. Addition of 0.2% BSA prevented NPs agglomeration and stabilized the systems at all studied conditions.

Thus, the data obtained indicate the interaction of both forms of glutathione with orthovanadate nanoparticles, which can affect the level and bioavailability of these molecules in living systems, as well as induce rearrangements in cellular glutathione-dependent antioxidant defense systems.

ACKNOWLEDGMENTS

This work was supported by National Academy of Sciences of Ukraine (Project № 0122U002636)

Nano-engineered Materials in Cosmetics, Safety Aspects: Data System "Rana"

Viktoriia Paientko[1, 2 *], Ewa Skwarek[1]

[1] *Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland (Poland)*
[2] *Chuiko Institute of Surface Chemistry, NAS of Ukraine (Ukraine)*
* payentkovv@gmail.com

Abstract ID #NRA-0605

Nanotechnology and nanomaterials are "trendy" and have made their way into cosmetics development. Some of the used nanomaterials are new (nanosomes, nano-gels and emulsions and etc.), the others are as old as the cosmetic industry itself (titania oxide, clays, silica etc.). At the same time safety of nanomaterials is an uneasy question of high importance[1]. Considering all issues related to the application of nanomaterials, a specialized data system "Rana" was developed – designed to store and systematize, calculate the development of cosmetics composition data, and determine their safety level. Unlike modern solutions in this area, this data system is completely isolated, which eliminates confidential data theft, has a strictly structured system of data input and output, and reduces the number of errors and time to master the system. The Firebase Realtime Database cloud database (Google technologies), was used for data storage. The safety of compound compositions can be predicted using the database. The program functions can be used to obtain quick answers about composition safety and to optimize the final composition. "Rana" is a new data system developed with the goal of a safety level prediction for nanomaterial-based compositions to support all the activities regarding the nanomaterials formulation in cosmetics industry engineering, bridging science, technologies, and high education

ACKNOWLEDGMENTS

The research leading to these results are supported by project NCN UMO-2022/01/4/ST5/00025

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Nanobiotechnology in Medicine: Medical Students' Awareness

Nataliia Inshyna *, Inna Chorna

Sumy State University (Ukraine)

* n.inshina@med.sumdu.edu.ua

Abstract ID #NRA-0609

Nanobiotechnology plays a crucial role in the development of new methods for diagnosis, prognosis, and treatment of various disorders. Nanomaterials have countless potential for application in many fields, particularly in pharmacy and biomedicine, tissue engineering, drug/gene delivery, development of medical implants for regeneration and healing of body tissues, and biological imaging [1-3]. Over the last 20 years, nanotechnology has become a common research trend. Most studies on nanobiotechnology have focused only on technical development. Previous studies on nanobiotechnology have not addressed the social aspects and public awareness of this field. The principal objective of this project was to investigate the level of awareness of medical students about nanobiotechnology in medicine, and to determine whether it is necessary to include nanomedicine and nanobiotechnology as academic courses in the medical curriculum.

Methods: A combined qualitative and quantitative methodological approach was used to determine students' awareness of and attitudes toward nanobiotechnology in medicine. We used focus group discussions as a qualitative approach [4] and a survey study as a quantitative method. A total of 110 survey questionnaires were completed by undergraduate medical students at Sumy State University (SumDU). The questionnaire consisted of the demographic profile of the participants, information regarding the source of knowledge of nanobiotechnology of the respondents, awareness questions about nanomedicine, and attitude-based items toward nanotechnology applications in medicine. The questionnaire data were analyzed using SPSS.

Results and discussion: The findings showed that most medical students were aware of nanobiotechnology. Overall, the majority of the students (52%) had a moderate or high level of awareness about the application of nanobiotechnology in medicine, 30% had the satisfactory level, and 18% - low level. The respondents reported the application of nanobiotechnology in oncology, dentistry, surgery, and orthopedics. At the same time, they did not know about the application of nanobiotechnology in tissue-specific clinical diagnostics and biomedical imaging. The research presented herein confirms that the medical curriculum should include nanobiotechnology in its academic course. Most medical students (77%) were interested in studying new nanomedicine and nanobiotechnology courses.

Undergraduate medical students in SumDU showed a satisfactory level of awareness and positive attitudes towards nanotechnology in medicine. The results of this study support the view that nanomedicine and nanobiotechnology could be essential components of the medical curriculum to help medical students become high-level professionals. The research results represent a further step toward developing modern medical education standards.

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Injectable Theranostic Platforms Based on Amino-Functionalized Magnetic SBA-15 Nanorods for Neurological Diseases

Zulema Vargas Osorio[1 *], Andrés Da Silva Candal[2], Yolanda Piñeiro[3], José Rivas[3], Martin Michálek[1], Dušan Galusek[4]

[1] *Centre for functional and surface functionalized glass, Alexander Dubček University of Trenčín, Študentská 2, 911 50 Trenčín, Slovakia (Slovakia)*
[2] *Clinical Neurosciences Research Laboratory, Health Research Institute of Santiago de Compostela (IDIS), Clinical University Hospital, Universidade de Santiago de Compostela, Santiago de Compostela, Spain (Spain)*
[3] *NANOMAG Laboratory, Institute of Materials, Applied Physics Department, Universidade de Santiago de Compostela, 15782, Santiago de Compostela, Spain (Spain)*
[4] *Joint Glass Centre of the IIC SAS, TnUAD, FChPT STU, Študentská 2, 911 50 Trenčín, Slovakia. (Slovakia)*
* zulema.vargas@tnuni.sk

Abstract ID #NRA-0610

A growing concern in neurology is associated with the increase in the number of cases related to Alzheimer's and Parkinson's diseases, as well as strokes, which occur more frequently and at increasingly young age. The situation is aggravated by the ageing of population. The development of novel theranostic materials that can act both as contrast agents and carriers of therapeutic molecules, providing simultaneously an efficient diagnosis and therapy, has thus gained significant attention [1]. Smart injectable SBA-15 nanorods-based nanocomposites coated by SPIONs covalently anchored by an amino-functionalized silica nanolayer have shown promise as a material for brain applications [2]. In this work, we use a degradable SBA-15 mesoporous silica as the support matrix with high drug loading capacity. Modification of the synthesis parameters allowed production of nanoscale SBA-15 rods with ordered and interconnected cylindrical pore channels [3]. The presence of a silanol-rich surface facilitated the anchorage of magnetite nanoparticles, which were selected due to their good biocompatibility and magnetic response [4]. The injectable theranostic nanoplatforms were characterized, showing a large surface area of 318 m2g-1 measured by N2 sorption and a functionalized surface characterized by elemental chemical analysis and 29Si MAS NMR. Preliminary in vitro and in vivo studies confirmed a high cellular uptake by brain endothelial cells up to 200 µg/mL particle concentration. No negative effect on liver or kidneys was observed after intravenous and intra-arterial injection into rats. Rhodamine B was incorporated to induce fluorescence properties into these complex nanostructures for future multimodal MRI/optical imaging applications.

ACKNOWLEDGMENTS

This item is a part of dissemination activities of project FunGlass.

This project has received funding from the European Union´s Horizon 2020 research and innovation programme under grant agreement No 739566.

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Synthesis and Analysis of Selected Physicochemical Properties of Clay/Hydroxyapatite/Clitoria Ternatea Composites with Doped SiO_2, TiO_2, ZnO_2 as an Additive to Cosmetics.

Klaudia Kowalska[1 *], Viktoriia Paientko[2, 3], Evgeny Demianenko[4], Ewa Skwarek[2]

[1] *Department of Radiochemistry and Environmental Chemistry Maria Curie-Sklodowska University (Poland)*
[2] *Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland (Poland)*
[3] *Chuiko Institute of Surface Chemistry, NAS of Ukraine (Ukraine)*
[4] *Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine (Ukraine)*
* klaudia.kowalska113@gmail.com

Abstract ID #NRA-0613

Due to its properties, i.e. biocompatibility, thermal stability and osteoconductivity, hydroxyapatite is the basis of the developing branch of biomedical technology. Natural admixtures are sought that can enrich the composite with the components we desire and enhance some of its properties [1]. The contemporary use of composites is not limited to biocomponents, but they are used more and more widely. According to the principles of "green chemistry", they represent a great potential not only for material engineering, but can also be used as heavy metal adsorbents [2,3]. Due to low toxicity of clay and hydroxyapatite, attempts were made to use the composite for the production of cosmetics and to establish closer cooperation with their producers [4].

The composite was obtained by mechanochemical synthesis of yellow clay, hydroxyapatite, silica, TiO_2, ZnO_2 with the addition of *Clitoria Ternatea*. Initially, the concentration of anthocyanins and chlorophyll in the samples was determined using UV/VIS spectrophotometry. The crystal structure of the samples was also analyzed and determined by X-ray diffraction (XRD). To determine the parameters of the porous surface structure of the samples, the method of low-temperature adsorption - nitrogen desorption (ASAP 24050) was used. Potentiometric titration and electrokinetic measurements were performed in the pH range of 5-11, in the basic electrolyte $NaNO_3$. The influence of ionic strength and pH on the following composite/NaCl interfaces was investigated, especially on: surface charge density and zeta potential. Theoretical calculations of the enthalpy of intermolecular complex formation were also made, thanks to which a potential model of the complex molecule was obtained. In addition, the toxicity and carcinogenicity of the obtained composites were tested.

The concentration of anthocyanins was between 230,99 μg/g and 904,09 μg/g. The highest concentration was obtained for the sample containing yellow clay, hydroxyapatite, zinc oxide and *Clitoria Ternatea*, and the lowest for the sample containing yellow clay fired at 200°C, hydroxyapatite, zinc oxide and *Clitoria Ternatea*. The concentration of chlorophyll was between 1045,35 μg/g and 9940,49 μg/g. The highest concentration was obtained for the sample with the composition of yellow clay, hydroxyapatite, zinc oxide, *Clitoria Ternatea*, and the lowest for the sample with the composition of yellow clay fired at 200°C, hydroxyapatite, titanium oxide, *Clitoria Ternatea*. The specific surface area for the tested samples was between 6 m^2/g and 15 m^2/g.

High concentration of anthocyanins and chlorophyll show good sorption properties of the composite, after analyzing the composites of yellow clay and hydroxyapatite with *Clitoria Ternatea*. The large specific surface area and the presence of pores allow for a wide range of applications as scaffolding for various types of plant additives in the cosmetics industry.

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Features of Electrical Properties of Nanocomposite Antimicrobial Polymeric Materials with Silver Nanoparticles

Eduard Lysenkov[1 *], Olexander Stryutsky[2], Iryna Lysenkova[1]

[1] *Petro Mohyla Black Sea National University (Ukraine)*
[2] *Institute of Macromolecular Chemistry, NAS of Ukraine (Ukraine)*

* ealysenkov@ukr.net

Abstract ID #NRA-0624

Polymer composite materials filled with metal particles are increasingly being used in global practice. The practical application of such materials is constantly growing, which is caused by the fact that they combine the optimal properties of polymers and inorganic particles. A special place among metal-polymer composites is occupied by materials with the inclusion of silver nanoparticles (AgNPs). Polymer nanocomposite materials containing AgNPs are widely used in medicine, pharmacy and food industry due to their unique antimicrobial properties. However, in order to create a promising bactericidal material, it is necessary to study other functional properties, in particular electrophysical ones. The aim of our work was developing novel antimicrobial nanocomposite materials and studying of their electrophysical properties. These properties are necessary in the case of creating antistatic and dissipative coatings that have an antimicrobial function.

The electrophysical properties of nanocomposite materials were studied using electrical impedance spectroscopy method and equivalent electrical cirquit simulation method.

Here we show the novel approach for creation of new antimicrobial polymeric nanocomposite materials based on polyethylene oxide (PEO) and study of their electrical properties. We have found that stabilized AgNPs significantly affect the electrical properties of the polymer matrix at relatively low concentrations of the nanofiller (~ 1%). At the same time, the electrical conductivity exhibits extreme behavior with increasing filler content in the system. It was determined that the greatest effect on the electrical properties of the studied systems is observed at a concentration of AgNPs equal to 1%. It is assumed that in systems based on PEO, there are two mechanisms of charge transfer: charge hopping in the crystalline phase of PEO and transfer provided by the segmental mobility of polyether chains in the amorphous phase of PEO. It was established that the aggregation processes of the filler and the proportion of the interfacial layer have a decisive influence on the electrical properties of PEO-based nanocomposite systems at low concentrations of AgNPs. It was found that with a filler content equal to 1%, the share of the interphase layer in the system is maximum. Nanocomposite with 1 % of AgNPs shows significant activity for Klebsiella, E. coli and Staphylococcus aureus.

We have studied the features of electrical properties of new materials with high antimicrobial activity. This approach allows us to develop new antimicrobial materials, based on various polymer matrices an additional nanofillers. The investigated materials with improved electrical properties in the future can be used as antimicrobial coatings, antimicrobial films with high antistatic and dissipative characteristics.

Bioinspired Adhesive Nanofibrous Hydrogel Demonstrates Synergistic Effect of Chemo-immunotherapy for Osteosarcoma Treatment

Wei Yuan Huang

(Taiwan)

Abstract ID #NRA-0644

Osteosarcoma (OS) is the most common primary malignant bone tumor. Although surgery and chemotherapy can relieve the symptoms and improve the outcome of patients, the local recurrence, metastasis and unresectable bone tumors are still clinical problems. In this study, a nanofibrous hydrogel composite is developed to synergize antitumor effect using chemotherapy as first line treatment modality followed by immunotherapy to clean residual tumors. The nanofibrous hydrogel is composed of two layers, an upper layer consisting of catechol-functionalized gelatin hydrogel and a lower layer made up of PCL-PEG/hyaluronic acid electrospun nanofiber matrix. Doxorubicin (DOX) is loaded in the upper layer for anticancer effect and mediates tumorigenic cell death, while immunomodulatory cytokines including interleukin-12 (IL-12) and interferon-gamma (IFN-γ) are complexed with polyelectrolyte complex nanoparticles (PCNs) in the lower layer to preserve the bioactivity and extend the release time from the hydrogel composite. In addition, the unique characteristic of this nanocomposite hydrogel is its adhesive patch application potential, allowing it to be wrapped around the bone tumor site for localized treatment to minimize side effect of systemic toxicity. The synergistic effects of DOX and cytokines were observed for anticancer and induction of immune responses both in vitro cell culture study and in vivo animal study. This composite may serve as a promising scaffold for applications in osteosarcoma therapy as well as other types of disease treatment.

Silicon Surface Sonomodification for Biointegration

Rada Savkina*, O. Y. Gudimenko, Vasyl Morozhenko, Oleksii Smirnov, Maria Smoliy

[1] *V.E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine (Ukraine)*

* rada.k.savkina@gmail.com

Abstract ID #NRA-0678

An important challenge in the development of semiconductor nanoelectronic systems for applications in biology is focused on their biocompatibility and reliability of the nano/bio interfacing. It can be solved by introducing functional groups at the solid surface which allow careful tuning its properties such as wettability, biocompatibility, electrical stability, corrosion resistance, and other. Complex and expensive chemical and plasma technological methods are employed for electronic materials biofunctionalization usually. In this report, we focus on the alternative pathway of the surface developing dealing with cavitation assisted methodology. This approach has many advantages over conventional methods as it is an environmentally friendly, simple, and low-budget process which allowed us to functionalize technologically relevant material such as silicon.
The properties of the Boron-doped p-type (100) Si samples and Si/TiO_2 structures subjected to cavitation impacts have been studied. It was found that high intensity (15 W/cm^2) and high frequency (1 ÷ 6 MHz) focused sonication of the samples investigated induces changes of the optical, electrical and structural properties of semiconductor surfaces confirmed by the results of X-ray difraction, as well as Raman and FTIR spectroscopy investigations. Besides, impedance and photovoltage spectroscopies were used for the sample's characterization. The complex stress state and phase transformations on the Si surface induced by acoustic cavitation are observed. We found that the cavitation processing results in formation CH_2-, CH_3-, and NH-terminated silicon surfaces with antireflection properties in the MWIR and NWIR spectral ranges. Besides, fabrication of a submicron silicon oxide layers as well as wollastonite/hydroxyapatite coating on silicon surface subjected to cavitation processing, are demonstrated under appropriate conditions. The obtained composite structure has demonstrated photoluminescence in the (500-800 nm) spectral range. Bioactivity of the ultrasonically processed substrates was confirmed by the hydroxyapatite formation on the Si surface after storage in simulated body fluid solution. This study shows the feasibility of using cavitation processing approach to fabrication both organic and calcium silicate/phosphate coatings on silicon in an attempt to improve its biointegration. Transferring our technology to the flexible polymer substrates and using SiO_2 as a long-lived, flexible biofluid barrier will, in our opinion, allow to advance in the field of developing flexible bioelectronic systems designed to interface to soft tissues of the human body [1].

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Ethical Issues of Nanomedical Research

Oksana Sulaieva *

Medical Laboratory CSD (Ukraine)

* o.sulaieva@csd.com.ua

Abstract ID #NRA-0680

Nowadays nanotechnologies have penetrated various fields of biomedicine providing fascinating opportunities to detect disease earlier and target drug delivery with minimal side effects [1]. Using nano-scale medications and gene therapy provides promises for the treatment of various illnesses, including inherited pathology, cancer, and neurodegenerative diseases. The development of nanosensors seems to be essential for effective disease monitoring and complications prevention [1]. The application of biomaterials for creating scaffolds for tissue engineering improved cells growth and their differentiation into functionally effective tissues that fueled the progress in regenerative medicine [2]. Besides, engineering of new molecular assemblers, reordering matter at a molecular or atomic scale, can impact repair or detection of pathologies [3]. Although nanotechnologies seem to revolutionize the healthcare system, their development and implementation possess potential adverse effects and unexpected events dangerous for personal health, society and environment that address the need for the proper ethical and regulatory framework. Herein the basic ethical issues of nanomedical research are discussed.

From the perspective of core bioethical principles (beneficence, nonmaleficence, autonomy, and justice) researchers running nanomedical studies have the ethical imperative to benefit the patient, to avoid or minimize harm, and to respect the values and preferences of the patient [4]. The safety of nanotechnologies and their impact on human health and the environment is the crucial ethical issues. This dictates responsible research conduct and human subject protection, appropriate research protocol review by IRB, proper risk-benefit assessments, relevant informed consent procedures and continuous monitoring of clinical study results [5]. The deploying of implantable nanodevices associated with sensitive health data collection can provoke privacy breach that requires adequate privacy protection and data security measures.

Nanotechnologies application for enhancement purposes, including cognitive improvement or cosmetic purposes, raises additional ethical questions related to fairness, societal values, and equitable distribution and availability of new nanomedical technologies. The adoption of nanotechnologies can potentially exacerbate healthcare disparities [4]. Distributive justice requires equal share according to needs and contribution, merit and free-market exchanges. Ensuring transparency in the development, testing, and deployment of nanotechnologies also encompasses the regulatory oversight and public engagement.

In conclusion, nanotechnologies application in biomedicine has the potential to revolutionize healthcare. However, nanomedical studies and the transfer of nanotechnologies to clinical settings should adhere to ethical and regulatory frameworks for ensuring the safety of individuals, society, and the environment.

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Ceramic-metal Nanocomposite Materials for Biomedical Applications

Svetlana Krivileva[1 *], Alexandr Zakovorotniy[2], Victor Moiseev[3], Ievgeniia Manoilo[2], Sergiy Kostenko[2]

[1] *National Technical University «Kharkiv Polytechnic Institute» (Ukraine)*
[2] *National Technical University – «Kharkiv Polytechnic Institute» (Ukraine)*
[3] *National Technical University Kharkiv Polytechnic Institute (Ukraine)*
* Svitlana.Kryvilova@khpi.edu.ua

Abstract ID #NRA-0696

In recent years, ceramic-metal nanocomposite materials (cermets) with biological activity have become widespread. They have important applications in modern medical technology, including prosthodontics, trauma and oncology surgery, and restorative medicine. Here we show that the most promising is the production of cermets of the calcium phosphate matrix-medical titanium composition by hot pressing, while the optimally selected ratio of the components of the calcium phosphate material and its structure ensure fusion with living bone in a given time frame with the restoration of the original histological structures and the germination of blood vessels. The use of cermets provides two tasks: improving the integration of foreign bodies with living bone tissue and combating re-implant infection. Both unresolved problems can lead to rejection of artificial products. The use of cermets, which cause a minimal inflammatory reaction, provides accelerated osseointegration due to the contact of the living bone exclusively with the root part, which has a calcium phosphate composition without the inclusion of foreign elements. The aim of this work was to study ceramic-metal nanocomposites for use in modern medical technologies, namely in orthopedic dentistry as intraosseous dental implants. The objects of study were cermets based on calcium phosphate bioceramics based on hydroxyapatite and medical grade titanium. Electron microscopy methods were used to study samples obtained under different pressing modes and different ratios of components in ceramics, and mechanical tests were also carried out. The possibility of introducing components with effective bactericidal properties into the composition of the calcium phosphate material to ensure an antimicrobial effect in the process of implant engraftment was studied. The developed ceramic-metal nanocomposites based on a calcium phosphate matrix and medical titanium (Ti Grade 5) can be used as highly effective and reliable intraosseous dental implants for fixed prosthetics in case of loss of a significant number of teeth.

Long Term Drug Delivery with Nanoparticles in the Treatment of Ocular Neovascular Diseases

Saliha Durak*, Ozlem Kutlu, Sibel Cetinel

Sabancı University (Turkey)

* salihadurak@sabanciuniv.edu

Abstract ID #NRA-0715

Nanoparticles have shown great potential as a drug delivery system for the treatment of neovascular ocular diseases. These diseases, such as age-related macular degeneration and diabetic retinopathy, are characterized by the growth of abnormal blood vessels in the retina that can cause vision loss. The current standard of therapy for neovascular ocular diseases involves administering monoclonal antibody-based anti-VEGF (anti-Vascular Endothelial Growth Factor) drugs via intravitreal injections on a periodic basis. The short half-lives of the drugs utilized in current treatment methods necessitate frequent injections, which can limit the effectiveness of the treatments. Hence, there is a need to develop new approaches for enhanced bioavailability and sustained and long-lasting delivery of anti-VEGF drugs.

The aim of this study was to utilize poly(glycerol sebacate) (PGS) nanoparticles to achieve an extended release of anti-VEGF drugs, with the objective of reducing the frequency of intravitreal injections required for treatment. Double emulsion solvent evaporation method was utilized for the synthesis of PGS nanoparticles with a size of approximately 150 nm and PDI less than 0.3. The encapsulation efficiency of nanoparticles loaded with anti-VEGF drugs was found to be 74%. The 30% drug release from nanoparticles in the first 2 months indicates that nanoparticles are a promising candidate for sustained drug release applications. Cell-viability studies showed that anti-VEGF drug-loaded nanoparticles did not exhibit toxicity to ARPE-19 cells, but they did exhibit anti-angiogenesis properties by inhibiting the growth of HUVEC cells in a concentration-dependent manner. The development of new-generation materials for the storage and preservation of anti-VEGF drugs, as well as their enhancement with prolonged release, will considerably improve the efficacy of long-term treatment strategies for ocular neovascular diseases.

Dextran-Graft-Polyacrylamide/Zinc Oxide Nanosystem does not Trigger Eryptosis

Anton Tkachenko[1 *], Anatolii Onishchenko[1], Volodymyr Yurievich Prokopiuk[1], Pavlo Virych[2], Nataliya kutsevol[2]

[1] *Kharkiv National Medical University (Ukraine)*
[2] *Taras Shevchenko National University of Kyiv (Ukraine)*
* as.tkachenko@knmu.edu.ua

Abstract ID #NRA-0731

Hemocompatibility of nanomaterials is an important step in the assessment of their safety due to the inevitable interactions of nanomaterials with blood upon their administration. A nanosystem composed of dextran-graft-polyacrylamide (D-PAA) and ZnO nanoparticles synthesized using zinc acetate as a precursor for nanoparticles (D-PAA/ZnO NPs (-OAc)) has been reported to show anti-cancer effects. However, its hemocompatibility is not fully tested. Eryptosis (Erythrocyte apoptosis or Red blood cell programmed death) is a type of apoptosis that occurs in injured erythrocytes (RBCs) due to various factors including hyperosmolarity, oxidative stress, energy depletion, heavy metals exposure or xenobiotics. Like apoptosis, eryptosis is characterized by cell shrinkage, membrane blebbing, activation of proteases, and phosphatidylserine exposure at the outer membrane leaflet. To test eryptosis parameters as an effective strategy to assess the hemocompatibility of newly synthesized nanomaterials. Erythrocytes incubated with D-PAA/ZnO NPs (-OAc) nanocomplex at concentrations 0-100-200-400 mg / L for 24 h were stained with Annexin V-FITC and 2',7'-dichlorodihydrofluorescein diacetate (H2DCFDA) with further flow cytometric analysis. Here We found that D-PAA/ZnO NPs (-OAc) nanocomplex does not trigger eryptosis, i.e. a suicidal regulated cell death of erythrocytes. In particular, incubation of the nanocomplex with blood (hematocrit 0.4%) for 24 h at concentrations 0-100-200-400 mg / L does not promote cell shrinkage (forward scatter signaling), phosphatidylserine externalization (Annexin V-FITC staining) or reactive oxygen species (ROS) generation (H2DCFDA staining), which are known to be hallmarks of eryptosis. Thus, our findings indicate that eryptosis is not triggered by D-PAA/ZnO NPs (-OAc) nanocomplex at concentrations demonstrating anti-cancer activity contributing to experimental evidence concerning the low toxicity of this nanocomplex. Furthermore, we believe that eryptosis can be widely used as a sensitive and reliable marker of nanomaterial hemocompatibility.

Cultured Fibroblasts-Based Assays Reveal Good Biocompatibility of Dextran-Graft-Polyacrylamide/Zinc Oxide Nanosystems

Volodymyr Prokopiuk[1 *], Anatolii Onishchenko[2], Nataliya Kutsevol[3], Pavlo Virych[3], Anton Tkachenko[1]

[1] *Kharkiv National Medical University (Ukraine)*
[2] *Research Institute of Experimental and Clinical Medicine, Kharkiv National Medical University (Ukraine)*
[3] *Taras Shevchenko National University of Kyiv (Ukraine)*

* v.yu.prokopiuk@gmail.com

Abstract ID #NRA-0732

The Food and Drug Administration has currently approved over 70 nanotechnology-based drugs. One of the factors that have contributed to limitations of clinical application of nanomaterials is their toxicity. Experimental evidence indicates that nanosystems synthesized from dextran-graft-polyacrylamide (D-PAA) and ZnO nanoparticles, which are produced with the help of either zinc acetate (D-PAA/ZnO NPs (-OAc)) or zinc sulphate (D-PAA/ZnO NPs (SO42-)) as precursors for nanoparticles, have anti-tumor activity in vitro. To consider their anti-cancer potential for further animal and clinical studies, it is primary necessary to study their toxicity. Our study aimed to assess the toxicity of dextran-graft-polyacrylamide (D-PAA) and ZnO nanoparticles against normal cells in vitro. Nanocomplexes were incubated with primary dermal rats embryonic fibroblasts for 24 h at 0-100-200-400-800 mg / L. Metabolic activity and viability was investigated using MTT and neutral red uptake assays, mobility by scratch test, proliferation – by population doubling time method. We demonstrate that both D-PAA/ZnO NPs (-OAc) and D-PAA/ZnO NPs (SO42-) nanocomplexes show low toxicity against fibroblasts. D-PAA/ZnO NPs (-OAc) nanocomplex neither reduced the viability of cells, nor affected their motility, evidenced by MTT and neutral red uptake assays, and scratch test, respectively. At the same time, MTT assay revealed that D-PAA/ZnO NPs (SO42-) nanocomplex diminished the viability of fibroblasts at 800 mg / L, while scratch assay showed that this nanocomplex negatively affected the migratory capacity of cells starting from 200 mg / L. Thus, our findings indicate that the use of zinc acetate reduces the toxicity of D-PAA/ZnO NPs nanocomplexes compared with zinc sulphate, however both complexes demonstrate good biocompatibility. This toxicological study suggests that D-PAA/ZnO NPs (-OAc) and D-PAA/ZnO NPs (SO42-) could be further investigated as anti-cancer drugs, since initial evaluation of their toxicity against normal dermal fibroblasts shows their good biocompatibility profile.

Biocidal Activity of Nanomaterials for Next-Generation Applications

Varaprasad Kokkarachedu *

Facultad de Ingeniería, Arquitectura y Diseño, Universidad San Sebastián, Lientur 1457, Concepción, Chile (Chile)

* prasad.kokkarachedu@uss.cl

Abstract ID #NRA-0735

Metal nanoparticles have been tremendously utilised as antibacterial and anticancer agents [1,2]. Although metal nanoparticles exhibit biocidal activity, but the drawback of toxicity on normal cells limits their clinical applications[3]. Therefore, improving the bioactivity and minimizing the toxicity of the nanomaterials is paramount for biomedical applications[4]. However, the design of nanomaterials with divalent ions and biomolecules (i.e. biomolecule curcumin, biopolymers) can improve the biosafety of the metal nanoparticles. In addition, the biogenic process can minimise the toxicity of innovative nanomaterials. This presentation addresses the importance of nanotoxicity nanomaterials, their development, and their applicability in clinical and 3-D printing applications. Additionally, our recent studies on biomolecule curcumin, biopolymer chitosan, and alginate influence on various metal nanomaterials and their mechanism are also discussed.

ACKNOWLEDGMENTS

Prof. Dr. Varaprasad Kokkarachedu acknowledges the Fondecyt Regular Project No: 1211118, ANID and Facultad de Ingeniería, Arquitectura y Deseno, Universidad San Sebastián, Chile.

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Immunological Properties of $T_2C_3T_x$ MXene

Sergiy Kyrylenko[1 *], Oksana Sulaieva[2], Zhanna Klishchova[1], Mykola Lyndin[1], Volodymyr Deineka[1, 3], Tetiana Shapochka[2], Anton Roshchupkin[1], Ilya Yanko[1], Yevheniia Husak[1], Oleksiy Gogotsi[4], Maksym Pogorielov[5, 6]

[1] *Sumy State University (Ukraine)*
[2] *Medical Laboratory CSD (Ukraine)*
[3] *Institute of Atomic Physics and Spectroscopy, University of Latvia (Latvia)*
[4] *Materials Research Center, Y-Carbon Ltd, Kyiv (Ukraine)*
[5] *Sumy State University, Sumy (Ukraine)*
[6] *University of Latvia, Riga (Latvia)*

* kyrylenk@gmail.com

Abstract ID #NRA-0752

MXenes are a family of 2D materials with unique physicochemical properties such as high surface area, excellent electrical conductivity and mechanical strength. Recently, MXenes have gained attention in biomedical applications. Thus, MXenes possess high optical energy to heat transfer coefficient which makes them excellent sensitizers for photothermal therapy [1]. In addition, MXenes have strong selective ability to adsorb various molecules, e.g. urea, which provides opportunity to design wearable dialysis devices for patients with kidney insufficiency [2]. Ability to modulate immune responses by MXenes has been shown via selective absorption of cytokines and bacterial toxins [3]. This opens a possibility that MXenes can impact release of cytokines and chemokines, modulating inflammation and reaction of immune cells including T- and B- lymphocytes. MXenes have also been shown to modulate specific antiviral response [4]. Additionally, MXenes have been preliminarily shown to enhance the activation of dendritic cells, leading to the production of a higher number of antigen-presenting cells, which still requires verification. Considering these findings, MXenes could provide substantial promises as immunotherapeutic agents for treating diseases such as cancer and autoimmune disorders. However, more research is required to understand better their immunological properties and potential applications in clinical settings. We postulate that MXenes can directly interact with immune cells. To investigate this option, we developed a system for cultivation of immune cells out of peripheral blood mononuclear cells (PBMC) isolated from donor blood. After 2 weeks in cultivation, some of the PBMCs get attached and acquire a characteristic macrophage-like morphology. In addition, they express CD31, leucocyte common antigen (LCA) and epithelial membrane antigen (EMA). We concluded that the PBMCs differentiate into macrophage lineages. We obtained the PBMC-derived macrophages on glass coverslips and investigate their interplay with T2C3Tx MXene. We previously showed that MXene could get associated with the cells in culture [1]. We also previously showed that MXenes interact with the CHO cells in-vitro. Currently we investigate whether the macrophages can recognize MXenes as foreign particles and phagocyte them. We hope that our experimental setup will answer the questions on possible activation of immune cells with MXenes and induction of expression of specific markers. In addition, we will use this system to investigate the fate of MXene after they get phagocytosed. We suggest that the cutting-edge techniques of single-cell mass cytometry by time-of-flight (CyTOF), imaging mass cytometry (IMC) and multiplexed ion-beam imaging by time-of-flight (MIBI-TOF) will be an ideal detection modality for simultaneous interrogation of multiple cellular parameters at the label-free single-cell level resolution [5].

ACKNOWLEDGMENTS

This work was supported by the Horizon Europe MSCA-2021-SE-01 project 101086184 MX-MAP; Ukraine MES grant "The mechanisms of MXene interactions with biological systems" ID: 0122U000784; and the Erasmus+ Jean Monnet Chair project 101085451 CircuMed.

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Design and Development of Curcumin-based Nano Fibrous Mats as Drug Eluting Stent Grafts for the Treatment of Coronary Diseases

Murtaza Najabat Ali*, Amna Aleem Khawaja, Bakhtawar Ghafoor, Zunaira Qureshi, Mariam Mir

National University of Science and Technology (Pakistan)

* murtaza.bme@hotmail.com

Abstract ID #NRA-0756

Neointimal proliferation after stent implantation may result in in-stent restenosis (ISR), which is a critical concern in the field of medicine. It results from the inflammatory reaction, proliferation of vascular smooth muscle cells (VSMC), thrombus formation and arterial recoil triggered by stent implantation (1). In this context, it is imperative to conduct research for finding effective solutions to avoid ISR. In this research, novel polyvinyl alcohol (PVA) nanofibrous mats loaded with curcumin extract were synthesized as drug eluting stent grafts using electrospinning technique. Curcumin extract, a natural antioxidant, anti-coagulant and anti-microbial agent (2) was incorporated in a blend of high and low molecular weight PVA which is a synthetic, non-toxic and biodegradable polymer (3). The developed nanofibrous mat was characterized using SEM, FTIR and XRD. The curcumin extract loaded PVA mats with varying drug concentrations were then subjected to in vitro analysis to investigate their antioxidant, antimicrobial, degradation, and drug release profile. Antioxidant activity and antimicrobial activity was highest for 0.65% w/w curcumin extract loaded PVA mats. The burst release of the drug was highest for 0.65% w/w curcumin and lowest for 2.19% w/w curcumin content. An initial burst drug release is required to avoid in-stent restenosis which is triggered after stent deployment. The required drug release was achieved with nanofibrous mat comprising of the lowest concentration of drug. In conclusion, the synthesized electrsopun nanofibrous films encapsulating curcumin extract showed significant antimicrobial and antioxidant activity. The results from degradation and drug release studies and the established anti-coagulant effect of curcumin extract in the literature suggest that the composition with lowest curcumin extract concentration could be utilized as potential candidate for coating drug eluting stents for treating coronary artery disease and avoiding in-stent restenosis.

ACKNOWLEDGMENTS

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

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Effect of Silver Nanoparticles Incorporation on Properties of Poly(lactic acid)/Chitosan Electrospun Nanofibrous Composite

Yuliia Varava[1 *], Kateryna Diedkova[2, 3], Yevheniia Husak[4], Yevhen Samokhin[1], Valeriia Korniienko[1], Baiba Zandersone[5], Baiba Krauze[5], Vladlens Grebnevs[6], Tatjana Tračevska[5], Maksym Pogorielov[2, 3], Viktoriia Korniienko[7, 1]

[1] *Biomedical Research Centre, Medical Institute, Sumy State University, Sumy (Ukraine)*
[2] *Sumy State University, Sumy (Ukraine)*
[3] *University of Latvia, Riga (Latvia)*
[4] *Sumy State University (Ukraine)*
[5] *University of Latvia (Latvia)*
[6] *Silesian University of Technology, Faculty of Chemistry (Poland)*
[7] *University of Latvia, Institute of Atomic Physics and Spectroscopy (Latvia)*
* yuliia.varava@gmail.com

Abstract ID #NRA-0758

Introduction. The development of biomaterials that combine the structural, chemical, and biological characteristics required to encourage tissue growth is vital for tissue engineering [1]. A combination of natural (Chitosan) and synthetic (PLA) polymers is a promising strategy that can allow the production of highly-effective scaffolds using electrospinning for tissue regeneration [2]. The presence of metallic nanofillers (silver nanoparticles) provides a modification of surface properties that can improve hydrophilicity and enforce the antibacterial properties of composite [3]. The aim is the evaluation of the structural and functional properties of Ch-PLA-AgNPs nanofibrous electrospun membranes depending on the concentration of incorporated AgNPs.

Materials and methods. Ch/PLA nanofibrous electrospun membranes were manufactured by electrospinning and followed by drop casting of AgNPs in different concentrations (400, 200, 100, and 50 µg/mL). Determining the colony count was carried out to evaluate the ability of the samples to inhibit bacterial growth at different time intervals of incubation (2, 4, 6, 8, and 24 hr) in the suspension of S. aureus and E. coli. The samples were analyzed on SEM, FT-IR spectrophotometer and video-based optical contact angle meter.

Results. SEM showed randomly oriented fibers. FT-IR and EDX confirmed that the AgNPs did not change the structure of the polymer. Nanofibers remained morphologically and structurally intact after loading with AgNPs. The incorporation of nanoparticles influenced the hydrophilicity of the membrane decreasing the contact angle twice up to 50°. The membranes doped with 400 and 200 µg/mL inhibited the growth of both microorganisms at 2, 4, and 6 hr points of the incubation. However, composite loaded with 100 µg/mL exhibited a noticeable antibacterial effect on E. coli at 2, 4, 6 hr points of co-cultivation. Otherwise, S. aureus strain was more resistant to samples with lower amounts (100 and 50 µg/mL) of nanoparticles within all time points of the experiment.

Conclusion. The results suggest that the Ch/PLA composites are potentially suitable for use as scaffolds for biomedical applications. Combined fabrication technologies have been employed to prepare composite scaffolds with improved properties, such as Ch/PLA electrospun nanofibers coated with AgNPs offering a new strategy for designing high-performance antibacterial biomaterials.

ACKNOWLEDGMENTS

This research was funded by HORIZON-MSCA-2021-SE-01-01 (Nr 101086441, ARGO), ERA-NET JPIAMR-ACTION JTC 2022 "Design and implementation of silver-based nanoparticles for combating antibiotic resistance" (VARIANT) and Latvian-Ukrainian Joint Programme of Scientific and Technological Cooperation «Implementation of 2D bi-layered nanomembranes for guided tissue regeneration in endo-perio lesions and periimplantitis».

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Impact of Silicates and Phosphates on the Properties of Anodized Magnesium Implants

Yevheniia Husak[1*], Anna Skoczylas[2], Natalia Waloszczyk[2], Maksym Pogorielov[3, 4], Wojciech Simka[2]

[1] *Sumy State University (Ukraine)*
[2] *Silesian University of Technology, Faculty of Chemistry (Poland)*
[3] *Sumy State University, Sumy (Ukraine)*
[4] *University of Latvia, Riga (Latvia)*

* evgenia.husak@gmail.com

Abstract ID #NRA-0761

The electrolyte composition and concentration are determine the ceramic coating structure and surface properties after the plasma electrolytic oxidation (PEO). Different ddditives into the base electrolyte system could provide formation of coatings with multifunctional properties, which is especially important for bioapplication [1]. Some research demonstrated processing of PEO coatings of Magnesium (Mg) implants in silicate- and phosphate-based electrolytes and shown that these anions enhance corrosion protection and the quality of the coating (porosity, thickness, microhardness) [2, 3]. However, there are no cocsensus about the better parameters of solution and PEO regimens for this purpose. Therefore, our research aims to understand the comprehensive interaction of silicates and phosphate anions to Mg implant surface properties after PEO for biological applications.

We elaborated four versions of sodium hydroxide based (5g/L) electrolyte for Mg implant PEO treatment: C1) 10g/L Na_2SiO_3, 10g/L Na_2HPO_4; C2) 10g/L Na_2SiO_3, 5g/L Na_2HPO_4; and C3) 10g/L Na_2SiO_3, 5g/L NaH_2PO_4; C4) 15g/L Na_2SiO_3, 10 g/L NaH_2PO_4. The PEO process was conducted under an impulse current up to a fixed voltage with use of a high-voltage power supply (PWR 800H, Kikusui, Japan). The coated sample's structure and their elemental composition were analyzed by scanning electron microscopy (SEM) equipped with energy-dispersive X-ray spectroscopy (EDX).

All surfaces had typical porous structure. Coatings C1, C2, and C3 contained tiny and evenly distributed pores with average sizes 0.07±0.12 µm, 0.05±0.11 µm, and 0.4±0.11 µm respectively at 200V. It is worth noting for samples C1, C3, C4 was applied higher voltage that course the rising of pore size value 0.13±0.33 µm (225V), 0.08±0.24 µm (250V), 0.10±0.21 µm (250V). The thickness of the PEO layers comprised up to 1,17µm. The elemental composition of Si and P, in atomic percentage, was around 4% and 1.7% for surfaces obtained at 200V. Whereas, voltage increasing raised the amount of the Si and P for all coatings, especially for C4 - 8% and 4%. The PEO coatings showed the wettability in the range 21° and 33°. Also, the influence type of phosphate on roughness was not noticed.

The set of results indicates that the surface morphology had equal characteristic for both type of electrolytes. However, samples obtained at higher voltage possessed more perfect surface. For completeness of the investigation, the next step will be conducting analysis the corrosion behavior of surfaces, due to all surfaces suitable for further bioinvestigation.

ACKNOWLEDGMENTS

Grant of Ministry of Education and Science of Ukraine, «Condition of mineralized tissues using new composites with Ag^+ and Cu^{2+} nanoparticles», 0121U100471

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The Structure of Nanocrystalline Calcifications from the Gallbladder

Roman Moskalenko[1,2*], Sergey Danilchenko[3], Andriy Stepanenko[2], Tattygul R Akhunbaeva[4], Roman K Kalmatov[4]

[1] *Ukrainian-Swedish Research Center SUMEYA, Medical Institute, Sumy State University, Sumy (Ukraine)*
[2] *Sumy State University (Ukraine)*
[3] *Institute of Applied Physics National Academy of Sciences of Ukraine (Ukraine)*
[4] *Osh State University (Kyrgyzstan)*

* r.moskalenko@med.sumdu.edu.ua

Abstract ID #NRA-0768

Pathological calcifications are commonly observed in gallbladder diseases such as cholelithiasis, gallbladder cancer, and porcelain gallbladder, which can lead to complications such as cholecystitis, pancreatitis, and biliary obstruction [1]. Therefore, investigating the morphology and physicochemical composition of gallbladder calcifications can provide insights into their formation mechanisms and potential treatment strategies [2,3]. Additionally, the information gathered from studying pathological calcification in the gallbladder can be applied towards developing new biomedical materials and identifying novel diagnostic markers for gallbladder diseases. This research has the potential to advance our understanding of gallbladder pathologies and improve patient outcomes. So far, we aimed to analyze the morphology of pathological biomineralization in GB tissue in ChL, GBC, and PGB.

We have analyzed 25 samples of GB calcifications (5 cases of PGB, 15 examples of ChL, and 5 cases of GBC with biomineralization) by histology (hematoxylin-eosin staining), histochemistry, X-ray diffraction, transmission electron microscopy, and scanning electron microscopy with EDS.

Here we present novel findings regarding the crystal phases of biominerals present in gallbladder (GB) pathologies. Our study reveals that hydroxyapatite is the predominant mineral found in intraparietal calcifications of porcelain gallbladder (PGB) and gallbladder cancer (GBC), while calcium carbonate with phosphate additives is the main component of stones from the GB cavity in cases of cholelithiasis (ChL). These results suggest distinct conditions, causes, and mechanisms underlying the formation of these different types of calcifications.

In particular, PGB and GBC share common features of calcification, characterized by dystrophy, necrosis, and cellular death in the GB walls, along with the occurrence of building materials for mineralization (calcium and phosphates). These observations are consistent with our previous studies of biomineral formations in other tissues, such as the aorta, thyroid, and prostate. We propose that local tissue damage and collagen fiber denudation may promote the formation of hydroxyapatite crystals, which are similar to those found in bone and synthetic biomaterials.

In contrast, calcification in ChL occurs within the GB cavity and is associated with calcium-containing concretions that are more resistant to mechanical destruction than organic stones. These calcium stones can take on various shapes and colors, ranging from snow-white to dark brown or black. Our research suggests that calcium carbonate with small amounts of nanocrystalline calcium phosphate phases (vaterite, dolomite) are the main components of ChL calcifications.

These findings provide a better understanding of the pathogenesis of GB diseases and may facilitate the development of new diagnostic markers and therapeutic approaches.

ACKNOWLEDGMENTS

This research has been performed with the financial support of grants of the Ministry of Education and Science of Ukraine No. 0112U100471, "Condition of mineralized tissues using new composites with Ag+ and Cu2+ nanoparticles".

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Refining the Thermal Decomposition Method for Semi-Continuous Production of Magnetic Iron Oxide Nanoparticles

Egon G. Höfgen *, Sulalit Bandyopadhyay

Partilce Engineering Centre, Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim (Norway)

* egon.hofgen@ntnu.no

Abstract ID #NRA-0780

Magnetic iron oxide nanoparticles (IONPs) have made the breakthrough from extensive research into manifold biomedical applications, such as drug delivery, hyperthermia therapy, biosensing and imaging. One successful example is the Norwegian SARS-Cov-2 test developed by our team, which utilizes silica coated IONPs in sample extraction.[1] With the rapidly increasing demand for IONPs rises the demand for efficient and scalable production methods. The synthesis via thermal decomposition offers excellent control over size, shape, crystallinity, and thus magnetic properties of the IONPs. Despite the widespread use of this method, it is predominantly employed as a batch reaction with inherent variability, limiting scalability and automatization which, however, are desired in commercial applications.

To address these limitations, we have successfully translated thermal decomposition into a semi-continuous process through optimization of chemical synthesis parameters. By doing so, we were able to produce spherical IONPs in the size range of 4.2 nm to 14.3 nm, with high monodispersity (8% PDI at 10.5 nm) and magnetic saturation close to bulk values, which are comparable to our batch experiments and literature.[2] Moreover, we were able to obtain anisotropic particles of varying shapes and sizes up to 100 nm by changing synthesis parameters instead of using additional chemicals.

Despite yielding high-quality particles, the hydrophobic nature of IONPs resulting from thermal decomposition impedes their direct biomedical application. This challenge was solved by employing established phase transfer methods. Through the thereby introduced carboxylic functionalities we achieve aqueous compatibility and high colloidal stability of the IONPs while maintaining their size, shape, and magnetic moment.

To conclude, our study demonstrates the successful translation of thermal decomposition into a semi-continuous process to produce high-quality IONPs with targeted properties and render them aqueously compatible, which is essential for biomedical applications such as nucleic acid extraction.

ACKNOWLEDGMENTS

The Research Council of Norway is acknowledged for funding this project (project number 327917) and the support of the Norwegian Micro- and Nano-Fabrication Facility, NorFab (project number 295864).

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DNA Comet Assay Points to Potential Genotoxicity of $T_2C_3T_x$ MXene

Zhanna Klishchova[1*], Inna Chorna[1], Anton Roshchupkin[1], Ilya Yanko[1], Ivan Baginskyi[2], Veronika Zahorodna[2], Iryna Roslyk[2], Oleksiy Gogotsi[2], Maksym Pogorielov[3, 4], Sergiy Kyrylenko[1]

[1] *Sumy State University (Ukraine)*
[2] *Materials Research Center, Y-Carbon Ltd, Kyiv (Ukraine)*
[3] *Sumy State University, Sumy (Ukraine)*
[4] *University of Latvia, Riga (Latvia)*

* kgeJP1990@gmail.com

Abstract ID #NRA-0794

MXenes are a class of two-dimensional materials widely used in various fields, including energy storage, environmental sensing, electronics and, most recently, in biomedicine. Like all new materials, concerns about their potential toxicity have been raised [1]. Several studies have investigated the potential toxicity of MXenes, including their ability to interfere with cell proliferation. These studies have shown mixed results, with some suggesting that certain types of MXenes may be toxic while others show no toxic effects [2]. Currently, there is limited information available on the potential genotoxicity of MXenes, and their impact on human health is not yet fully understood. Therefore, further research is required to determine their harmful effects, if any, and to develop strategies to limit any potential negative impact.

The DNA comet assay [3], also known as single cell gel electrophoresis, is a sensitive technique used to detect DNA damage in individual cells. It involves embedding cells in agarose, lysing the cells to release their DNA, and subjecting the DNA to electrophoresis. This causes the DNA to migrate away from the nucleus and form a comet-like shape under fluorescent staining. The extent of DNA damage can be quantified by assessing the length, shape and intensity of the comets with longer and more intense tails indicating greater levels of damage. DNA damage can occur due to various factors such as exposure to radiation, environmental pollutants, toxins and chemicals.

It is largely assumed that MXenes are generally well tolerated by living cells. We and others observed that T2C3Tx MXene directly interacts with cells in various cell cultures [4]. We also showed that the MXene gets associated with the CHO cells in-vitro.

To investigate if MXenes show potential genotoxicity, we treated B16F10 mouse melanoma cells with 6.25, 25 and 100 µg/ml of T2C3Tx MXene for 4 hrs, washed the MXene away and further cultivated of the cells under standard conditions for additional 3 days. We then performed alkaline DNA comet assay. We found that incubation of the cells with T2C3Tx MXene induced robust appearance of DNA comets in a dose-dependent manner. The degree of the induction of the DNA comets did not correlate with the apparent lack of toxicity of the MXene. We hypothesized that the observed effect could be an artifact of the assay. To assess that possibility, we performed the assay with the heat-killed cells and showed that the killed cells did not display the DNA comets in presence of MXene. This confirmed, that induction of the DNA comets with MXene requires metabolically active cells. We also showed that parameters of the DNA comets induced by MXene differ from those induced by H2O2. Currently, we conduct thorough investigation of the observed phenomenon of induction of the DNA comets with MXenes. This can have substantial implications in the development of new technologies in regenerative biomedicine using novel nanomaterials [5].

ACKNOWLEDGMENTS

This work was supported by the Horizon Europe MSCA-2021-SE-01 project 101086184 MX-MAP; Ukraine MES grant "The mechanisms of MXene interactions with biological systems" ID: 0122U000784; and the Erasmus+ Jean Monnet Chair project 101085451 CircuMed.

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Side-by-Side Electrospun PCL-Ag NPs/CA-Lavender Oil Janus Nanobelt as Potential Wound Dressing

Meng-Long Wang[1, 1], Deng-Guang Yu[2], Sim Wan Annie Bligh[1 *]

[1] *School of Health Sciences, Caritas Institute of Higher Education (Hong Kong)*
[2] *School of Materials and Chemistry, University of Shanghai for Science and Technology, Shanghai (China)*
* abligh@cihe.edu.hk

Abstract ID #NRA-0805

Wound dressing with multifunction has been explored by many technologies. Side-by-side electrospinning was conducted by utilizing a specially designed Janus spinneret and preparing a PCL/CA Janus belt with Ag NPs on the PCL side and lavender oil (LO) on the CA side. The morphology and inner structure of prepared Janus nanobelts were observed by scanning electron microscope (SEM) and transmission electron microscope (TEM). Found that the products tend to form Janus nanobelt shape and have a rough surface with many pores. The physic states of raw materials and nanobelts were detected by X-ray diffraction (XRD). The compatibility within nanobelt was explored by Fourier transform infrared spectroscopy (FTIR). Characteristic peaks of each polymer can be found in the curve of nanobelts. Water contact angle tests showed that the Janus nanobelt has hydrophobic properties at around 120°. An antibacterial test was also conducted and observed a certain antibacterial performance in eliminating Escherichia coli. Ag NPs and linalool from LO can both provide antibacterial properties. Through this specially designed Janus spinneret, robust side-by-side electrospinning processes can be implemented with appropriate solutions and Janus fibers with good function can be obtained.

Multifluid Side-by-Side Electrospun Tri-layer Janus Fiber with Different Spinnable Solutions

Meng-Long Wang[1, 1 *], Deng-Guang Yu[2], Sim Wan Annie Bligh[1]

[1] *School of Health Sciences, Caritas Institute of Higher Education (Hong Kong)*
[2] *School of Materials and Chemistry, University of Shanghai for Science and Technology, Shanghai (China)*
* mwang@cihe.edu.hk

Abstract ID #NRA-0806

Electrospinning processes have been developed for many years. However, there are problems in preparing Janus fibers by side-by-side electrospinning processes. In this study, a special designed eccentric Janus spinneret was used to conduct tri-fluid side-by-side electrospinning process. This process utilized one spinnable solution to drive two unspinnable solutions and PVP/PVP-CA/CA tri-layer Janus fiber was successfully obtained. The prepared tri-layer Janus fiber has a smooth surface and distinguished inner structure as evidenced by scanning electron microscope (SEM) and transmission electron microscope (TEM). The forming process of tri-layer fiber and advantages of eccentric Janus spinneret would be presented. The tri-fluid side-by-side electrospinning system can be a robust platform in preparing multi-channel Janus fibers. These nanofibers can be used for many applications, such as drug delivery systems, catalytic carriers and photoluminescence.

Ultrafine-grained Bioabsorbable Zn Composite Stabilized by Nanometric ZnO Dispersoids

Martin Balog[1 *], Moara Marques de Castro[2], Jaroslav Capek[3], Peter Svec[2], Martina Takacova[4], Lucia Csaderova[4], Eva Sedlackova[4], Eliska Svastova[4], Andrea Skolakova[3], Drahomir Dvorsky[3], Jan Pinc[3], Vojtech Hybasek[5], Jiri Kubasek[5], Peter Krizik[1], Jacek Skiba[6]

[1] *Institute of Materials and Machine Mechanics, Slovak Academy of Sciences (Slovakia)*
[2] *Centre of Excellence for Advanced Materials Application, Slovak Academy of Sciences (Slovakia)*
[3] *Institute of Physics of The Czech Academy of Sciences (Czech Republic)*
[4] *Biomedical Research Center, Institute of Virology, Slovak Academy of Sciences (Slovakia)*
[5] *Department of Metals and Corrosion Engineering, University of Chemistry and Technology (Czech Republic)*
[6] *Institute of High Pressure Physics, Polish Academy of Sciences (Poland)*
* martin.balog@savba.sk

Abstract ID #NRA-0809

This study addresses the problem of intrinsic microstructural and mechanical instability of Zn-based biometals. It introduces a new concept of stable Zn based material, which is demonstrated for the particular model: the bioabsorbable in-situ Zn+ZnO metal matrix composite (MMC) manufactured by the consolidation of fine atomized high purity Zn powder by hydro-extrusion (HE). The detailed microstructural characterization and evaluation of its mechanical properties are presented. Post-processing stability, deformation and strengthening mechanisms, corrosion, and in-vitro biological behavior are pursued. A small fraction (4.75 vol.%) of ZnO nanodispersoids with the average size of ~136 nm formed in situ from passivating films present on Zn powder during HE, and are embedded in the refined Zn structure with an average grain size of ~750 nm. The ZnO dispersoids evenly distributed at Zn grain boundaries stabilize the grain structure by Zener pinning action during deformation and after annealing held at 100 °C for 24 h. The Zn+ZnO MMC shows superior mechanical properties (YS0.2 = 143 MPa, UTS = 153 MPa, ductility = 39%) than those reported for pure Zn materials. Immersion of the Zn+ZnO MMC in DMEM results in a corrosion rate of 0.018 ± 0.002 mm·y-1, which complies with the desirable standard rate for biodegradable materials. Both gravimetric and electrochemical corrosion tests suggest that the Zn+ZnO MMC and cast Zn reference reach a similar degradation rate after the first week of immersion. In-vitro cyto/genotoxicity assays performed using DMEM diluted extracts (25%) of the Zn+ZnO MMC and cast Zn incubated with L929 cells yield in a comparable and non-toxic response. The Zn+ZnO MMC induces a small but still significant bacteriostatic activity.

ACKNOWLEDGMENTS

The work was supported by the following projects: i) SRDA APVV-20-0417, ii) ITMS 313021T081 "Building-up Centre for advanced materials application of the Slovak Academy of Sciences" supported by Research & Innovation Operational Programme funded by the ERDF, iii) 21-11439K by Czech Science Foundation, iv) CzechNanoLab Research Infrastructure supported by MEYS CR (LM2023051), and v) SOLID21 - CZ.02.1.01/0.0/0.0/16_019/0000760 Operational Programme Research, Development and Education financed by European Structural and Investment Funds and by the Czech Ministry of Education, Youth and Sports. Dr. M. M. de Castro acknowledges Štefan Schwarz Support Fund.

Use of Magnetic Particles in MRI Thermometry

Zbigniew Celinski[1 *], Josh Stoll[1], Yu Hao[1], Robert Camley[1], Dorota Lachowicz[2], Angelika Kmita[2], Marek Przybylski[3], Janusz Hankiewicz[4]

[1] *Department of Physics and Energy Science, University of Colorado Colorado Springs (United States)*
[2] *Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology (Poland)*
[3] *Faculty of Physics and Applied Computer Science, AGH University of Krakow, 30-059 Krakow, Poland (Poland)*
[4] *University of Colorado, Colorado Springs Center for the Biofrontiers Institute (United States)*
* zcelinsk@uccs.edu

Abstract ID #NRA-0813

Magnetic resonance imaging (MRI) is a critical component in many medical procedures. For example, treating cancer during MRI guided thermal ablations requires real-time, spatially and thermally accurate temperature maps. We have demonstrated the effectiveness of using magnetic particles within a medium as MRI temperature sensors [1-5]. In studied phantoms, we have correlated the temperature dependent magnetic properties of particles with the nuclear magnetic relaxation times T_1, T_2, and T_2* of water or silicone hydrogen nuclei. We have acquired MRI images of the phantoms using both, the gradient echo method, which is sensitive to local magnetic field inhomogeneities (T2*), and the spin echo method which is sensitive to T_2 relaxation time. For example, embedding ferrite nanoparticles into an agarose gel allowed us to acquire strongly temperature-dependent MR images. The presented results indicate the possibility of using, in the future, the developed technique during MRI guided cryoablation and laser ablation.

ACKNOWLEDGMENTS

This research was supported by National Science Foundation SBIR grant #1843616 and the gift from the Kairos Ventures as well as by the Polish National Agency for Academic Exchange, project No. PPI/APM/2018/1/00049/U/001.

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Transformation of Frequency Dispersion of Electrical Parameters of Liver Tissues Depending on Its Storage Temperature.

Taras Pryimak*, Dmytro Chervinko, Ivan Gasyuk

Vasyl Stefanyk Precarpathian National University (Ukraine)

* pryimak.tr@gmail.com

Abstract ID #NRA-0815

The article discusses the temporal frequency transformation characteristics of electrical parameters of liver tissues during its storage in the temperature range of 2-35 °C. Changes in direct current conductivity, frequency dispersion of the real component of conductivity and tangent of dielectric loss angle in the frequency range of 0.01 Hz -100 kHz (alpha dispersion range) are considered in this article. The relationship between the transformation of temperature-time dependences of electrical parameters and the degree and nature of morphological changes in biological tissue has been established. In particular, it is shown that the local values and the monotonicity direction of the polarization relaxation-time function in the studied frequency range of electrical impedance spectra measurement can serve as a criterion for the degree and type of destructive changes in liver tissues when it is stored in an air atmosphere at different temperatures.

From Cancer Research to Antiviral Research: a Journey with 2D Materials

Açelya Yilmazer *

Department of Biomedical Engineering, Faculty of Engineering, Ankara University, Stem Cell Institute (Turkey)

* ayilmazer@ankara.edu.tr

Abstract ID #NRA-0820

Graphene and 2D materials have attracted a lot of attention in cancer research since their discovery, especially in cancer research. Thanks to their extraordinary properties, we have been using them to diagnose cancer, delivery chemotherapeutics or exert anti-tumor activities through various mechanisms. The COVID-19 pandemic has shown the success of nanotechnology in combating with viruses in different applications including the development of vaccines or personal protective equipment (PPE). Among these nanotechnology-based systems, two-dimensional (2D) materials with intrinsic physiochemical properties can efficiently favor antimicrobial activity and maintain a safer environment to protect people against pathogens. During this presentation, the antiviral studies performed using 2D materials will be discussed by shedding light on how these materials can reduce the chance of infection effectively. 2D materials can be used alone or combined for the disinfection process of microbes, antiviral or antibacterial surface coatings, air filtering of medical equipment like face masks, or antimicrobial drug delivery systems. At the same time, they are promising candidates to deal with the issues of conventional antimicrobial approaches such as low efficacy and high cost. Specific attention will be also provided in order to suggest new approaches to develop and design novel antimicrobial agents using 2D materials for combating global infectious diseases in the future.

Investigation of the Therapeutic Potential of $T_2C_3T_x$ MXene in the in-ovo Model

Sergiy Kyrylenko[1], Vyacheslav Oleksandrovych Kukurika [1 *], Artem Shmatkov[2], Volodymyr Deineka[1, 3], Zhanna Klishchova[1], Roman Moskalenko[4, 1], Oleksandr Solodovnyk[1], Ivan Baginskyi[5], Veronika Zahorodna[5], Iryna Roslyk[6], Oleksiy Gogotsi[5], Maksym Pogorielov[7, 8]

[1] *Sumy State University (Ukraine)*
[2] *Sumy State University (Ukraine)*
[3] *Institute of Atomic Physics and Spectroscopy, University of Latvia (Latvia)*
[4] *Ukrainian-Swedish Research Center SUMEYA, Medical Institute, Sumy State University, Sumy (Ukraine)*
[5] *Materials Research Center, Y-Carbon Ltd, Kyiv (Ukraine)*
[6] *Researcher at Materials Research Centr, Y-Carbon Ltd, Kyiv (Ukraine)*
[7] *Sumy State University, Sumy (Ukraine)*
[8] *University of Latvia, Riga (Latvia)*

* kukurikav25@gmail.com

Abstract ID #NRA-0837

MXenes are a class of two-dimensional nanomaterials that have shown promising therapeutic potential in various biomedical applications [1]. Their high surface area and unique chemical properties make them ideal for drug delivery systems, bioimaging and biosensing. MXenes have been studied for their ability to deliver cancer and anti-inflammatory drugs, with promising results in preclinical studies. We and others showed that T2C3Tx MXene have substantial potential to be used as a photosensitizer to develop an efficient protocol for photothermal therapy (PTT) of cancer using a pulsed infrared laser [2]. However, further research is needed to fully understand their therapeutic potential and to develop MXene-based medical products.

The in-ovo model is widely considered as an ethical and cost-effective alternative to traditional animal based testing methods. It offers an in-vivo setting to study effects of various treatments, drugs or conditions on developing embryos within a fertilized egg [3].

Melanoma is a type of skin cancer that can spread quickly to other parts of the body if not detected and treated early. Risk factors for melanoma include exposure to UV radiation from the sun or tanning beds. Melanoma incidence is on the rise in developed societies due to increasing exposure to the sun on the resort beaches without proper sunscreen protection. Melanoma can be a plausible target for treatment with the PTT approach because it is a superficial tumor which is relatively easily accessible to infrared laser irradiation. We postulated that melanoma cells could be used the in-ovo model to investigate the conditions for efficient PTT in-vivo using MXene as a photosensitizer.

For our experiments with development of a PTT protocol for treatment of melanoma we chose chicken embryos as a suitable in-ovo xenograft model [4]. The B16F10 mouse melanoma cells were cultivated in DMEM/F12 medium with 10% FBS under standard conditions. We engrafted 2 to 3 mln of the cells onto the chorioallantoic membrane (CAM) after 6-7 days of incubation of fertilized chicken eggs. We used silicone rings to position the cell suspension onto the CAM. To increase the efficiency of forming tumors we used a quick 20-sec irritation of the CAM with a filter paper soaked in 70% ethanol just before engrafting. After additional 6-7 days post-engraftment, the tumors reached 2-3 mm in size. Histological and immunohistological analyses confirmed that the formed xenograft tumors were indeed related to melanoma. We then engrafted in-ovo the melanoma cells treated with T2C3Tx MXene. We irradiated the tumors with the pulsed infrared laser through the opening in the egg shell 20-22 mm in diameter. One day after irradiation, we fixed the tumors in buffered formalin and subjected them to both histological and immunohistological analyses. We currently investigate the conditions for efficient PTT protocol of melanoma using chicken embryos as the in-ovo xenograft model.

ACKNOWLEDGMENTS

This work was supported by the Horizon Europe MSCA-2021-SE-01 project 101086184 MX-MAP; Ukraine MES grant "The mechanisms of MXene interactions with biological systems" ID: 0122U000784; and the Erasmus+ Jean Monnet Chair project 101085451 CircuMed.

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Multifluid Side-by-Side Electrospun Tri-Layer Janus Fiber with Different Spinnable Solutions

Sim Wan Annie Bligh[1 *], Deng-Guang Yu[2], Meng-Long Wang[1]

[1] *School of Health Sciences, Caritas Institute of Higher Education (Hong Kong)*
[2] *School of Materials and Chemistry, University of Shanghai for Science and Technology, Shanghai (China)*
* abligh@cihe.edu.hk

Abstract ID #NRA-0842

As potential drug carrier, nanofibers have attracted much attention. An important fiber-obtaining technology, electrospinning has been developed for many years. Herein, a multichannel fiber with side-by-side structure was developed, which can be a potential carrier for loading more than one drug in different channels [1,2]. In this presentation, the formation process of structure fiber will be addressed, which can provide a robust platform for various drug delivery systems. A specially designed eccentric side-by-side spinneret was used to conduct a tri-fluid side-by-side electrospinning process and utilized two spinnable solutions to drive one unspinnable solution. Polyvinylpyrrolidone (PVP) and cellulose acetate (CA) were used to prepare PVP/PVP-CA/CA tri-layer Janus fiber, as shown in the figure below. The prepared tri-layer Janus fiber has a smooth surface and distinguished inner structure, as evidenced by scanning electron microscope (SEM) and transmission electron microscope (TEM). Composite nanofiber shows 799 ± 183 nm diameter. The forming process of tri-layer fiber and the advantages of eccentric Janus spinneret was discovered. By utilizing the interaction between working solutions, many other unspinnable solutions can be applied in this process, which will widely extend the range of solutions that can be used. The tri-fluid side-by-side electrospinning can be a useful technology for preparing multi-channel fibrous drug delivery systems with various drugs loaded.

ACKNOWLEDGMENTS

This work was supported by the Hong Kong Research Grant Council (No. UGC/FDS11/P01/21) and the Natural Science Foundation of Shanghai (No.20ZR1439000). SWAB thanks the support of Institutional Strategic Grant of the Caritas Institute of Higher Education (ISG190101).

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Side-by-Side Electrospun PCL-Ag NPS/Ca-Lavender Oil Janus Nanobelt as a Potential Wound Dressing

Meng-Long Wang[1, 1 *], Deng-Guang Yu[2], Sim Wan Annie Bligh[1]

[1] *School of Health Sciences, Caritas Institute of Higher Education (Hong Kong)*
[2] *School of Materials and Chemistry, University of Shanghai for Science and Technology, Shanghai (China)*
* mwang@cihe.edu.hk

Abstract ID #NRA-0843

Electrospinning as a convincing technology in preparing nanofiber materials, has been developed to provide a lot of schemes in preparing fibrous membrane wound dressings. For the purpose of carrying different ingredients on the nanofiber, multichannel fibers with core-shell and/or Janus structures were developed. Lan et al. [1] coaxial electrospun PVA@PCL nanofiber with ε-poly(L-lysine) on the shell and tea polyphenols on the core. The results showed that ε-poly(L-lysine) on the shell side has a good antibacterial activity against E. coli and S. aureus. Dong et al [2] used Isatis root as the antibacterial ingredient and loaded it into PVP electrospun nanofiber. Ji et al. [3] prepared Janus fibrous wound dressing and loaded Rana chensinensis skin peptides (RCSPs) and silver nanoparticles (Ag NPs) into different sides. It is a combination of antibacterial performance and promotion of wound healing function. The aim of this work is to investigate different antibacterial active reagents in the novel Janus nanobelt for improved antibacterial performance.

Herein, side-by-side electrospinning was conducted by utilizing a specially designed Janus spinneret and prepared PCL/CA Janus nanobelt with Ag NPs on the PCL side and lavender oil (LO) on the CA side. Briefly, two working solutions were pumped into different channels of the spinneret through two pumps. Two working solutions would contact each other before they form Taylor cone. A Janus Taylor cone can be observed, and another two stages including straight jet and bending and swing were followed. Finally, solvent will be removed from working fluid, solidified into fiber materials, and collected by the collector. The flow rate of each solution was kept at 1.0 mL/h. Ambient temperature and humidity were 20 ± 3°C and 60 ± 5°, respectively. The high voltage applied was 12.0 kV. And collecting distance was kept at 20 cm.

According to scanning electron microscope (SEM) images, the products tend to form a Janus nanobelt shape and have a rough surface with many pores. The transmission electron microscope (TEM) image shows a clear side-by-side structure based on the grey level difference (Figure 2). The X-ray diffraction (XRD) patterns prove the successful loading of Ag NPs. Fourier transform infrared spectroscopy (FTIR) curves show the uniform dispersion of LO. Water contact angle tests showed that the Janus nanobelt has hydrophobic properties at around 120°. Antibacterial tests were also conducted and observed 14.55 ± 1.81 mm inhibition zones in eliminating Escherichia coli. Ag NPs and linalool from LO can both provide antibacterial properties. A synergistic effect should happen within the prepared Janus nanobelt. Through this specially designed Janus spinneret, robust side-by-side electrospinning processes can be implemented with appropriate solutions and Janus fibers with good function can be obtained.

ACKNOWLEDGMENTS

This work was supported by the Hong Kong Research Grant Council (No. UGC/FDS11/P01/21) and the Natural Science Foundation of Shanghai (No.20ZR1439000). SWAB thanks the support of Institutional Strategic Grant of the Caritas Institute of Higher Education (ISG190101).

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Potential Energy of Interaction Between Nanoparticles in the Concept of Effective Susceptibility

Valeri Lozovski[1 *], Taras Vasyliev[2], Mariia Babiichuk[3], Yelyzaveta Stuzhuk[3]

[1] *Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *National Taras Shevchenko University of Kyiv (Ukraine)*
[3] *Institute of High Technologies Taras Shevchenko National University of Kyiv (Ukraine)*
* v.lozovsk@gmail.com

Abstract ID #NRA-0866

The idea of the influence of self-consistency on the formation of the repulsive part of the interaction potential between two nano-particles was described in [1]. The method of calculation of adsorption potential is based on finding the ground state of the system of two nanoparticles by variate of the free energy over the dipole momentum at the particles. The effective susceptibility as the linear response to the external field [2] in a natural way occurs as the result of the findings. We calculated the adsorption potential and the effective susceptibilities for the simple case of system of two spherical nanoparticles with shells. It was shown that the interaction between the nanoparticles depends on the configuration of the nanoparticles system.

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Invasive and Non-invasive Neural Interfaces

Yael Hanein *

School of Electrical Engineering, Tel Aviv University (Israel)

* yaelha@tauex.tau.ac.il

Abstract ID #NRA-0869

Neural engineering is an emerging interdisciplinary field of research implements engineering techniques to investigate the function and manipulate the behavior of the central or the peripheral nervous systems. A primary overreaching goal of neuro-engineering research is to counter neuro-degenerative conditions and to improve diagnostics in neurodegeneration. In this talk I will present innovative electronic approaches for interfacing with the brain, focusing on nanomaterials and their integration into novel devices. Primarily, I will discuss devices designed to interface with the retinal [1] and devices that can help diagnostics and treatment in neuro-degenerative diseases such as Parkinson's disease [2-4]. In the domain of retinal interfacing, we have explored various materials including carbon nanotubes, nanorods and organic pigments to facilitate improved interfacing. In the domain of skin electronics, we have explored various carbon and PEDOT inks. In both applications, expansive electrophysiological investigations will be presented to demonstrate the validity of technology performances.

ACKNOWLEDGMENTS

This research was supported by an Israel Science Foundation (ISF) and ERC (FUNMANIA, 2007– 2013 and OuterRetina, 2023-2028) Grants.

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Tightly Packed Gold Nanoparticle Ensembles for Plasmonic Sensing Applications

Attila Bonyár[1, 2 *], Tomáš Lednický[3], Rebeka Kovács[1, 2], Shereen Zangana[1, 2]

[1] *Department of Electronics Technology, Faculty of Electrical Engineering and Informatics, Budapest University of Technology and Economics, Egry József u. 18, H-1111 Budapest (Hungary)*
[2] *Wigner Research Centre for Physics, Budapest (Hungary)*
[3] *Central European Institute of Technology, Brno University of Technology, Purkyňová 123, 612 00 Brno (Czech Republic)*

* bonyar.attila@vik.bme.hu

Abstract ID #NRA-0872

Recent developments in the fabrication technologies of plasmonic nanomaterials enable their effective utilization in advanced bioanalytical concepts, such as LSPRi and SERS. Localized surface plasmon resonance imaging (LSPRi) promises the possibility of high-throughput biomolecule sensing integrated into miniaturized point-of-care (PoC) devices. Surface-enhanced Raman spectroscopy (SERS) is a promising ultrasensitive method in which the Raman scattering signal strength of molecules, absorbed on the surface of metallic nanoparticles with intensive near-fields, is enhanced with several orders of magnitude. Both techniques require nanoparticles or nanostructures, preferably bound to a solid surface. Besides, the sensitivity of both methods depends on the intensity of the plasmon field around the particles, which can be enhanced by utilizing plasmonic coupling between closely packed nanoparticles.

In this talk, the importance of plasmonic coupling in the optimization of plasmonic sensor performance will be highlighted and illustrated with numerical simulation results. In a previous experimental work [1], a fabrication technology was presented to create tightly packed nanoparticle arrangements on large surface areas (in the cm^2 range), where the size (diameter, D_0) and interparticle distance (D) of the nanoparticles can be controlled in the $0.1 < D/D_0 < 0.8$ range. In the talk, the application of this novel AuNPs – epoxy surface nanocomposite for the label-free detection of short DNA fragments with LSPR and SERS methods will be demonstrated and discussed [1, 2].

ACKNOWLEDGMENTS

This work was partially supported by the Nanoplasmonic Laser Fusion Research Laboratory project (NAPLIFE) financed by the National Research and Innovation Office (2022-2.1.1-NL-2022-00002) and by the Eötvös Lóránd Research Network (ELKH), Hungary. Project no. TKP2021-EGA-02 has been implemented with the support provided by the Ministry of Culture and Innovation of Hungary from the National Research, Development and Innovation Fund, financed under the TKP2021-EGA funding scheme. A. Bonyár is also grateful for the support of the Hungarian Academy of Engineering and the "MICHELBERGER MESTERDÍJ" Scholarship. Tomáš Lednický acknowledges the CzechNanoLab Research Infrastructure supported by MEYS CR (LM2018110) and support granted by the Ministry of the Interior of the Czech Republic under No. VJ01010123.

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Towards Femtosecond Laser-induced Periodic Surface Structures in Developing Functional Surface Properties

Iaroslav Gnilitskyi[1, 2 *]

[1] *"NoviNano Lab" LLC, Lviv (Ukraine)*
[2] *Department of Applied Physics and Nanomaterials Science, Lviv Polytechnic National University, Lviv (Ukraine)*
* iaroslav.gnilitskyi@novinano.com

Abstract ID #NRA-0873

Surface morphology is a key factor in controlling the wetting, mechanical, chemical and biological properties of a surface. The surface morphology is mostly performed with well-established lithography techniques However, these techniques have a lot of drawbacks. The alternative can be lasers, especially ultrashort lasers, which offer a potentially simple and low-cost alternative. Surface modifications by lasers with a pulse duration in the femtosecond range have recently attained a lot of attention due to nonthermal ablation mechanisms [1]. Femtosecond pulses have also been exploited to induce periodic surface structures known as laser-induced periodic surface structures (LIPSS), firstly observed in 1965. These sub-micro and nanostructures are already used and have a potential to be applied in numerous fields, including holography, photonics, wettability and medicine [2]. The advanced method to generate LIPSS – HR (highly-regular) – LIPSS has been presented in 2016 [3]. HR-LIPSS allows fabrication of extremely uniform nanostructures, with excellent long-range repeatability.

Alongside with HR-LIPSS the ultrashort laser light by tuning of parameters allows to form a broad range of nano and microstructures. The period of structures can be changed by tuning angle of incidence for laser light or by changing a laser wavelength. The height and morphology are strongly dependent on laser fluence while direction of structures can be tuned by optics configuration.

In this study, the most recent applications of femtosecond laser surface modification including burst mode regime will be presented.

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Nanostructured Materials and Surfaces for Biomedical Applications

Natalia Beshchasna *

Fraunhofer Institute for Ceramic Technologies and Systems IKTS (Germany)

* natalia.beshchasna@ikts.fraunhofer.de

Abstract ID #NRA-0876

Inventions in nanotechnology widen the scope of the approaches for the development of new medical technologies, including those for atherosclerosis treatment. The process of atherosclerotic plaque formation and the accompanying molecular and cellular events create numerous opportunities for affecting them by nanoparticles (NPs). By attaching antibodies, proteins, peptides, or other ligands to their surface, NPs can be targeted to single or multiple receptors that are expressed on the surface or inside of an atherosclerotic plaque. Different processes, markers, and cells have been manipulated using NPs to achieve desired therapeutic effects.

Nanofeatures such as laser-induced periodic surface structuring of stents surface has been demonstrated to improve the reendothelialization properties of stents by influencing their interaction with cells. Another interesting approach is related to the effect of nano- and microstructuring on the corrosion resistance of metallic stents. Using functionalized nanomaterials improved biocompatibility, antithrombotic, antiinflammation and antimicrobial properties of medical implants e.g. stents can be achieved. Nanostructured surfaces provide unique properties for drug-delivery function and for release of the active substances from the implant surface.

The proposed invited talk will consider different aspects of the application of nanomaterials and nanostructured surfaces for biomedical applications.

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Nanoscopic Sensors in the World of Cancer Research

Larysa Baraban *

Institute of Radiopharmaceutical Cancer Research, Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), 01328 Dresden (Germany)

* l.baraban@hzdr.de

Abstract ID #NRA-0881

Immunotherapy using CAR-T cells is a new paradigm technology for cancer treatment. To avoid severe side effects and tumor escape variants observed for conventional CAR-T cells approach, adaptor CAR technologies are under development, where intermediate target modules redirect immune cells against cancer cells. In this work, silicon nanowire field effect transistors are used to assist in the development of target modules for an optimized CAR-T cell operation. Focusing on a library of seven variants of E5B9 peptide that is used as CAR peptide epitope, we performed multiplexed binding tests in serum using nanosensor chips. Peptides have been immobilized onto the sensor to compare the signals of transistor upon titration with anti-E5B9 antibodies. Correlation analysis of binding affinities and sensitivities enabled a selection of best candidates for the interaction between CAR and target modules. Finally, cytotoxic functionality of CAR-T cells in combination with the selected target modules were successfully proven. Our results open the perspective for the nanobiosensorics to go beyond the early diagnostics in the field of clinical cancer research, and paves the way towards personalization and efficient monitoring of the immunotherapeutic treatment, where the quantitative analysis with the standard techniques is not an option.

ACKNOWLEDGMENTS

The financial support from the European Research Council (ERC) in frames of a Consolidator Grant (ImmunoChip, 101045415) is greatly acknowledged.

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Exploring the Evolution of Nanometric Titanium Oxide Layers in Real-time During Immersion of Titanium Alloys in the Physiological Fluids

Agata Sotniczuk[1, 2 *]

[1] *NOMATEN Centre of Excellence, National Centre for Nuclear Research, A. Sołtana 7, 05-400 Otwock-Swierk (Poland)*
[2] *Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw (Poland)*
* Agata.sotniczuk@ncbj.gov.pl

Abstract ID #NRA-0885

Titanium and its alloys are one of the most widely used materials for the permanent implants such as joint or dental replacements [1]. This is associated to the advantageous combination of mechanical and functional properties such as corrosion resistance. Corrosion response is governed by the properties of the air-formed nanometric oxide layers that can be tailored by the microstructure and/or chemical composition of the substrate material. Typical procedures that are used to evaluate corrosion behavior of biomedical materials include standard electrochemical tests such as EIS or CV and ion-release measurements such as ICP-MS. These procedures give us useful information about the overall corrosion response. However, in order to obtain direct information what material's features are responsible for observed behavior, it could be necessary to visualize corrosion response for the selected micro-areas of the material's surface. This study presents how to gain this knowledge by using local techniques such as scanning electrochemical microscopy (SECM).

ACKNOWLEDGMENTS

SECM tests were funded by the European Union Horizon 2020 research and innovation program under Grant Agreement No. 857470 and from the European Regional Development Fund via Foundation for Polish Science International Research Agenda PLUS program Grant No. MAB PLUS/2018/8.

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MXene-cell Interactions: Influence of Size and Protein Corona Formation

Kateryna Diedkova[1,2 *], Evelina Bebre[2], Una Riekstina[2], Iryna Roslyk[3], Ivan Baginskyi[3], Veronika Zahorodna[3], Oleksiy Gogotsi[3], Maksym Pogorielov[1, 2]

[1] *Sumy State University, Sumy (Ukraine)*
[2] *University of Latvia, Riga (Latvia)*
[3] *Materials Research Center, Y-Carbon Ltd, Kyiv (Ukraine)*

* katefei93@gmail.com

Abstract ID #NRA-0886

MXenes is a new 2D nanomaterials that intensively investigated towards biomedical applications, including anti-cancer photo-thermal therapy, antibacterial agents, effective sorbents, and as additives for tissue engineering constructions. To date, over 30 stoichiometric MXenes have been experimentally produced, in addition to dozens of solid solution MXenes. They produced with variations in shape, size and surface chemistry that can significantly influence to their toxicity and final effects [1]. The toxicity of nanomaterials depends on their specific physicochemical properties, and it is therefore important to characterize the hazard potential of new nanomaterials such as MXenes [2]. Other very important problem related to nanomaterials during in-vivo application is formation of "protein corona" – the layer of proteins over the material that can significantly affect nanomaterials properties. The aim of our research was to evaluate biocompatibility of Ti_3C_4 MXenes with different lateral size and after the formation of protein corona.

Ti_3C_4 MXenes with lateral size 180, 600, 1000 and 3000 nm provided by Materials Research Center (Kyiv, Ukraine) as suspension in DI. Z-potential and MXenes' size was measured using Zetasizer Nano ZS system before and after the co-incubation in DMEM with 10% of Fetal Bovine Serum to assess the protein corona formation. Human keratinocytes (HaCaT), primary dermal fibroblasts, and murine melanoma cell line (B16F10) were used to assess the biocompatibility and cell-MXene interaction in standard and serum-free conditions to evaluate influence of material size and protein corona.

We found 2-fold increase of Z-potential following MXenes incubation with the serum supplemented cell culture media due to the formation of "protein corona". This leads to decreased stability of MXene solution that could affect their application as a pharmacological substance. MXenes without "protein corona" exhibit higher cell toxicity against B16F10 cell line due to higher cell penetration ability related to the smaller particle size and surface properties. The HaCaT cell line is more sensitive to MXene biomaterial compared to the B16F10 cell line due to higher proliferation rate of melanoma cells, and the toxic effects of MXene nanoparticles on HaCaT cells are equally manifested both in the presence and absence of protein corona. Our findings demonstrate the importance of controlling the nanomaterials parameters before the biomedical application to avoid possible side effects and complications.

ACKNOWLEDGMENTS

This research received support from the Horizon Europe MSCA-2021-SE-01 project 101086184 MX-MAP and from the Ukraine MES grant "The mechanisms of MXene interactions with biological systems" ID: 0122U000784.

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Identification of Pathogenic Fungus on Biosurface Using Optical Coherence Tomography Combined with Laser Speckle Contrast Imaging

Eglė Vansevičiūtė[1], Rimantas Daugelavičius[1], Simona Vaitkienė[1], Mikus Melderis[2], Roman Viter[2], Mindaugas Tamošiūnas[1, 2 *]

[1] *Department of Biochemistry, Faculty of Natural Sciences, Vytautas Magnus University, Vileikos 8, Kaunas LT-44404 (Lithuania)*
[2] *Institute of Atomic Physics and Spectroscopy, University of Latvia, Jelgavas 3, Rīga, LV-1004 (Latvia)*
* mindaugas.tamosiunas@lu.lv

Abstract ID #NRA-0887

The spread of infectious diseases caused by human fungal pathogens occurs through contacts with contaminated biosurfaces. The use of optical imaging techniques presents a potential solution for fast and accurate detection of pathogens at the macro scale level. Up to date, the commercial interferometric imaging systems have been developed with optical coherence tomography (OCT) and speckle imaging equipment integrated [1]. In this study, spectral domain OCT and laser speckle contrast imaging (LSCI) techniques were tested in a bi-modal set up for structural imaging of *C. albicans* clinical isolates (11017, 1251, 1368), obtained from patient's ascitic fluid at the Republican Hospital of Panevėžys (Lithuania) and prepared under controlled laboratory conditions at their mature biofilm stage.

The presence of *C. albicans* biofilm on cell culture plate surface could be identified through the distinct multi-scattering effect observed in B-can images, by using Telesto II (Thorlabs, USA) OCT equipment. The height of the upper envelope of the OCT image (< 40 μm) suggested the presence of approximately 6-7 layers of stacked C. albicans cells within the biofilm. While OCT imaging enabled clear identification of pathogens on the optically transparent cell culture plate surface, other tested biosurfaces, such as polycaprolactone (PCL) prepared w/wo selenium (Se) nanoparticles exhibited the scattering as their dominant optical property. This resulted in obscured identification of *C. albicans* biofilm presence, due to the multi-scattered signals from *C. albicans* and PCL become merged and also exceed the depth of the PCL biosurface.

In the proposed bimodal set-up, the LSCI equipment [2] which was custom assembled and applied sequentially, provided ability to detect the microbial biofilm presence on the cell culture dish and on the PCL biosurfaces, and to assess the response of *C. albicans* cells to antifungal treatment. Our results showed a strong correlation between the speckle contrast parameter (s/<I>) obtained through LSCI and the optical density values obtained from *C. albicans* biofilm sample using MTT assay. The optical density values from the MTT assay are commonly used as a measure of cell metabolic activity, which is often interpreted as an indicator of cell viability. In detail, our results showed that a decrease in speckle contrast values correlated to a decrease in *C. albicans* biofilm cell viability estimated 24 hours after antifungal treatment using fluconazole and nystatin, with concentrations ranging from 0.5 to 256 μg/ml. Notably, the speckle contrast remained unchanged when antifungal treatments were administered at lower drug concentrations. We foresee that integration of speckle-based techniques into OCT imaging platforms would enable studying the biofilm-related phenomena, including biofilm growth on the biosurfaces, and aid in the development of antimicrobial strategies.

ACKNOWLEDGMENTS

The research was funded by cluster research project P-G-22-08 "The resistance of pathogenic microbes and biofilms to antimicrobial compounds" at Vytautas Magnus University, Kaunas, Lithuania).

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Labeling of Cellular Targets Using Promising Two-Photon Contrast Agent Based on Sorted Nitrogen-Doped Graphene Quantum Dot–Polymer Conjugates Exhibiting Excitation-Wavelength-Independent Photoluminescence

Wen-Shuo Kuo *

Center for Allergy Immunology and Microbiome (AIM), China Medical University Hospital, China Medical University, Taichung 404 (Taiwan)

* activesitess@gmail.com

Abstract ID #NRA-0893

In this study, high-uniformity sorted nitrogen-doped graphene quantum dots (N-GQDs) with different sizes displayed the phenomenon of excitation-wavelength-independent photoluminescence emission. The electronic properties and mechanisms involved in quantum-confined photoluminescence can serve as the foundation for the application of oxygenated graphene in photonics, and biology. Further, the sorted N-GQDs were then conjugated with polyethylenimine exposed under two-photon excitation, resulting in good biocompatibility and a higher photoluminescence quantum yield, two-photon absorption, two-photon luminescence emission, absolute cross section of two-photon excitation, ratio of radiative decay rate/non-radiative decay rate, stability and a change in lifetime that could be served as promising two-photon contrast probes. These exceptionally bright, highly photostable, and multiplexing-compatible sorted N-GQD-polymer materials are suitable for employment as fluorescence probes in biological and biomedical applications for analyzing multiplexed targets.

Molecularly Imprinted Polypyrrole Electrochemical Sensor for L. Monocytogenes Detection

Maksym Pogorielov[1, 2 *], Viktoriia Korniienko[1, 2], Kateryna Diedkova[1, 2], Vilma Ratautaite[3], Arunas Ramanavicius[3]

[1] *Institute of Atomic Physics and Spectroscopy, University of Latvia (Latvia)*
[2] *Biomedical Research Centre, Medical Institute, Sumy State University, Sumy (Ukraine)*
[3] *Department of Nanotechnology, State Research Institute Center for Physical Sciences and Technology (Lithuania)*
* m.pogorelov@med.sumdu.edu.ua

Abstract ID #NRA-0895

The detection of bacterial pathogens is of utmost importance for ensuring food safety and preventing outbreaks of foodborne illnesses. Among these pathogens, Listeria monocytogenes is a common cause of infections with high mortality rates, particularly among vulnerable populations1. Therefore, the development of a rapid, sensitive, and specific detection method for L. monocytogenes is essential to ensure the safety of food products.

In recent years, molecularly imprinted polymers (MIPs) have emerged as a promising sensing platform for the selective and sensitive detection of various analytes, including bacteria2. Specifically, polypyrrole (PPy), a conducting polymer, has garnered significant attention for its excellent conductivity, stability, and biocompatibility, making it ideal for use in electrochemical sensors.

Within this context, we developed a novel electrochemical sensor based on molecularly imprinted polypyrrole for the specific detection of L. monocytogenes. The sensor was designed by imprinting L. monocytogenes cells into a PPy matrix, resulting in specific binding sites that recognize and selectively capture the target cells. To optimize the sensor's performance, we varied the synthesis conditions of the MIP-PPy and the electrochemical parameters.

The developed sensor exhibited excellent sensitivity and specificity towards L. monocytogenes, with a detection limit of 10 CFU/mL. Additionally, it demonstrated good stability and reproducibility, establishing it as a reliable and robust tool for detecting L. monocytogenes in food samples. Overall, the MIP-PPy electrochemical sensor we have developed holds significant potential for the rapid and specific detection of L. monocytogenes, contributing to the enhancement of food safety and public health.

ACKNOWLEDGMENTS

Research was funded under the CFLA project "Jauna fotoluminescences platforma Listeria monocitogēnu noteikšanai" (1.1.1.5/21/A/001).

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Size and Concentration Dependence of Antimicrobial Activity for Copper Nanoparticles

Yuliia Varava[1 *], Valeriia Korniienko[1, 2], Rafal Banasiuk[3], Roman Moskalenko[4, 5], Maksym Pogorielov[2, 1], Viktoriia Korniienko[2, 1]

[1] *Biomedical Research Centre, Medical Institute, Sumy State University, Sumy (Ukraine)*
[2] *Institute of Atomic Physics and Spectroscopy, University of Latvia (Latvia)*
[3] *NanoWave, Wroclaw (Poland)*
[4] *Ukrainian-Swedish Research Center SUMEYA, Medical Institute, Sumy State University, Sumy (Ukraine)*
[5] *Sumy State University (Ukraine)*

* yuliia.varava@gmail.com

Abstract ID #NRA-0896

Copper nanoparticles (CuNPs) possess significant antibacterial properties, which have been extensively studied and recognized due to lower rates of microbial resistance compared to conventional antibacterial agents [1]. The multi-targeted mechanism of action and the rapid killing ability of CuNPs make it difficult for bacteria to develop resistance. The antibacterial properties have led to their exploration for various biomedical applications including the development of antimicrobial coatings. Although CuNPs exhibit strong antimicrobial activity, antibacterial potential depending on their size needs to be carefully evaluated. The aim of current research is to determine the minimum inhibitory concentration of CuNPs towards Gram-positive and Gram-negative strains depending on their size.

Two types of CuNPs with the same composition (provided by NanoWave Co., Poland) were studied. Nanoparticle size was measured using Zetasizer Nano ZS system. Minimum Inhibitory Concentration (MIC) by following the broth microdilution method established by CLSI. Determination of the minimum inhibitory concentration CuNPs was performed on *Enterococcus faecalis, S. aureus, S. epidermidis, P. aeruginosa, E.coli*.

Depending of synthesis ability, the size of CuNPs ranged from 89 nm (Sample 1) to 1464 nm (Sample 2). Sample 1 at a concentration of 127 µg/mL demonstrated an inhibitory effect against *S. aureus, S. epidermidis, P. aeruginosa*, and *E. coli*. Whereas Sample 2 demonstrated an inhibitory effect against only *S. epidermidis* and *P. aeruginosa* bacterial strains at the same concentration. *Enterococcus faecalis* was resistant to both samples at mentioned concentration.

An evident size effect on antibacterial mode was observed. Samples with a smaller nanoparticle size have better antibacterial properties. Copper nanoparticles at a concentration of 127 µg/mL can be considered a promising antibacterial agent with antibacterial activity against Gram-positive and Gram-negative bacteria.

ACKNOWLEDGMENTS

This research was funded by Latvian-Ukrainian Joint Programme of Scientific and Technological Cooperation «Novel copper-loaded wound healing patches with advanced regeneration capacity and antibacterial effect».

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TRACK 12

“THEORY & MODELING”

Formation of Single-Domain Structures In $BaTiO_3$ Upon Phase Transition

Olha Mazur[1*], Leonid Stefanovich[1], Ken-ichi Tozaki[2]
[1] *Branch for Physics of Mining Processes of the M.S. Poliakov Institute of Geotechnical Mechanics (Ukraine)*
[2] *Chiba University (Japan)*

* o.yu.mazur@gmail.com

Abstract ID #TM-515

Static and dynamic properties of perovskite ferroelectrics, which demanded in photovoltaics and photonics, are determined by the state of their domain structure1. Classical methods for controlling the domain ordering process are limited by technological issues and size effects. The use of self-assembling mechanisms under highly nonequilibrium conditions is very promising for obtaining single-domain and regular domain structures with a submicron period. However, this process is random and significantly depends on the prehistory of the sample2. Here we show that the initial inhomogeneity of the system under certain conditions determines the nature of the evolution of the domain structure. We found that only a polydomain state is formed in a barium titanate crystal when the weak external hydrostatic pressure $p < 19$ MPa is imposed on the sample. A strong pressure $p > 19$ MPa leads to the suppression of the ferroelectric phase and the formation of a single-domain structure in systems with low and high initial inhomogeneity, respectively. We found an expansion of the range of admissible pressures for the monodomainization of the system with an increase in the value of its initial dispersion of polarization. We show that it is not necessary to use "ideal" crystals to obtain single-domain structures. The high initial inhomogeneity of the system, which depends on the quenching rate and concentration of defects, can be an auxiliary tool for controlling the domain ordering. These results will be useful in preparing experiments under highly nonequilibrium conditions, where it is difficult to maintain the temperature and pressure values. Controlling the initial inhomogeneity of the sample by the quenching rate and alloying expands the possibilities for sample monodomainization. This will improve the methods for obtaining stable single-domain structures for modern device making, including high-efficiency solar cells3.

ACKNOWLEDGMENTS

This work was funded by the project № 9918 of the IEEE program "Magnetism for Ukraine 2022" supported by the Science and Technology Center in Ukraine (STCU) together with the Institute of Magnetism NASU and MESU, on behalf of the IEEE Magnetic Society.

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A Role of Diffusion of Adatoms Between Layers In Nano-Structured Thin Films Growth at Condensation

Alina Dvornichenko[1*], Vasyl Kharchenko[2], Dmitrii Kharchenko[2]
[1] *Sumy State University (Ukraine)*
[2] *Institute of Applied Physics National Academy of Sciences of Ukraine (Ukraine)*

* a.dvornichenko@mss.sumdu.edu.ua

Abstract ID # TM -516

Nanostructured thin films are extensively utilized in various areas of materials science to enhance the physical and chemical properties of materials. They find applications in magneto-resistive sensors, memory devices, optical and communication devices, quantum dot lasers, and detectors, playing a significant role in the rapid advancement of miniaturized electronic devices due to their unique properties and functional abilities such as giant magnetoresistance, controlled optical emission, high efficiency in photovoltaic conversion, and ultra-low thermal conductivity. To optimize the specific properties of nanostructured thin films for modern nano-electronic devices, different methods of film fabrication are employed including deposition from the gas phase and ion-plasma devices. The results of theoretical and experimental studies indicate that by using different materials, nanostructures of various types and sizes can be grown during the deposition process due to the combined effects of quasi-chemical reactions and interactions between the adsorbed. We perform theoretical studies of the formation and growth of adsorbate surface structures during condensation from the gas phase in the framework of the reaction-diffusion model. The main aim is to discuss an influence of the diffusion of adatoms between layers on the processes of adsorbate redistribution on the substrate. We show that an increase in the vertical diffusion coefficient leads to a decrease in the concentration of the adsorbate on the first growing layer, the realization of first-order transitions and reversible processes of adsorbate ordering on the substrate. With the help of numerical simulations, we demonstrate that in a limited range of values of the coefficient of vertical diffusion of adatoms between layers, its increase leads to a morphological transformation in the structure of the surface layer from separated holes in the adsorbate matrix (nano-holes) toward separated adsorbate structures on the substrate (nano-dots). The results obtained in the work can be useful for explaining the experimental data on the change in the morphology of the growing thin film during condensation.

Computer Simulation of Transition Metal Nitrides Thin Film Deposition

Dmytro Shyrokorad[1], Oleksandr Goncharov[2, 3 *], Ivan Kolinko[2], Svetlana Goncharova[2], Grygoriy Kornich[1]

[1] *National University "Zaporizhzhia Polytechnic" (Ukraine)*
[2] *Sumy State University (Ukraine)*
[3] *Institute of Materials Science, Slovak University of Technology in Bratislava, Trnava (Slovakia)*

* o.goncharov@mss.sumdu.edu.ua

Abstract ID # TM -517

Transition metal nitrides (TMN) thin films exhibit unique properties due to their combination of metallic, ionic, and covalent chemical bonds[1]. These properties make them applicable in a wide range of technologies, such as cutting industry, superconductors, semiconductors, magnetic materials, optics etc [2]. At the same time, a large number of parameters that must be controlled complicates the process of obtaining the film nanostructures with given physical and mechanical characteristics (hardness, modulus of elasticity, plasticity index) [3,4]. Thus, building robust models for preliminary investigation of the structure of thin films under different deposition regimes becomes an actual problem. Here we show some results of molecular dynamics simulation of transition metal nitrides films sputtering deposition, in particular, TiN film deposition on the iron substrate. The nucleus of the whisker, that forms columnar structure of the TiN coating, was observed. The Ti and N atoms tended to form NaCl-like structure with Ti atoms occupy octahedral sites, coordinating six N atoms. Computer simulations of such atomic systems make it possible to achieve the desirable nanostructure by setting appropriate sputtering conditions. We position our work as a starting point for the extension of the model to the other transitional metal nitrides, borides, and carbides. In addition, further increase of the simulation time intervals will lead to obtain the evolution of the column from the nucleus. In this regard, using temperature-accelerated and hyperdynamics approaches in the frameworks of accelerated dynamics methods looks promising due to realistic simulation of the time intervals between subsequent elementary acts of a particle deposition on the surface and final thin film deposition times.

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Dynamical Symmetry Breaking in Magnetic Systems.

Jaroslav Tobik *
Institute of Electrical Engineering, Slovak Academy of Sciences (Slovakia)

* jaroslav.tobik@savba.sk

Abstract ID # TM - 550

The symmetry of magnetic bodies is also reflected in the symmetry of their energy landscape. The process of symmetry breaking is a process where a state uniquely determined by some external parameter is transformed into a state of lower symmetry, i.e. into some degenerate state. Lower symmetry states are two or more energetically degenerate states at the same value of the control parameter. The symmetry broken states can be transformed amnong each other using some symmetry operation. As an example we can mention vortex core nucleation in magnetic dots in decreasing in-plane field, or emergence of the chiral state in magnetic dot in decreasing out-of-plane field. Although these proceses seems to be examples of the spontaneous symmetry breaking, we show that outcome of these processes can be predictable and not random. The controlability of the final symmetry-broken state is determined by magnetization dynamics, as it will be demonstrated on several simple and more complex systems.

ACKNOWLEDGMENTS

This work was performed during the implementation of the project Building-up CEMEA SAS, ITMS project code 313021T081 supported by Research \& Innovation Operational Programme funded by the ERDF . We also acknowledge funding from the Slovak Grant Agency APVV (grant number APVV-19-0311(RSWFA)) and grant VEGA 2/0177/21.

Analysis of Temperature Fields In FGM Macro/Nano Solids by Moving Finite Element Method

Ladislav Sátor *, Miroslav Repka
Institute of Construction and Architecture, Slovak Academy of Sciences (Slovakia)

* ladislav.sator@savba.sk

Abstract ID # TM -570

Within the classical theory of heat conduction the size of the specimen is not reflected. However, experiments have shown that in smaller samples that are nano/micro-sized, there are observable the size effect of various phenomena. By incorporating the higher-order gradients of primary field variables into the constitutive relationships, it becomes possible to explain these size effects within the generalized theory of continua. This paper deals with the higher-grade theory of heat conduction in micro/nano solids with functionally graded material (FGM) properties. Making use the variation principles, the mathematical formulation of the boundary value problems is derived within higher-grade theory of heat conduction, i.e. the governing equation and the physically admissible boundary conditions are derived. Applying the developed formulation for FGM solid structures we can derive rather complex governing equation with variable coefficients and higher order derivatives of field variables. It is well known the high order derivatives of field variables can lead to decreasing of accuracy of the numerical solution. To eliminate this problem the decomposition of the original governing partial differential equation (PDE) into the system of PDEs with lower order derivatives is proposed. For the numerical implementation the novel Moving Finite Element approximation method is utilized. Several numerical simulations are devoted to study the influence of micro-length scale parameter as well as the parameters of gradation of material parameters on the temperature field.

ACKNOWLEDGMENTS

The financial support of the Slovak Research and Development Agency under the contract No. APVV-18-0004 and VEGA 2/0061/20 are greatly acknowledged.

Computational Studies of Atomic and Electronic Structures of Phosphate-Molybdate and Phosphate-Tungstate-Vanadate Glass-Ceramics

Yuriy Hizhnyi[1 *], Vitalii Chornii[2, 1,] Serhii Nedilko[1, 3], Kateryna Terebilenko[1], Yaroslav Zhydachevskyy[3]
[1] *Taras Shevchenko National University of Kyiv (Ukraine)*
[2] *National University of Life and Environmental Sciences of Ukraine (Ukraine)*
[3] *Institute of Physics Polish Academy of Sciences (Poland)*

* hizhnyi@gmail.com

Abstract ID # TM -641

Computational modeling of atomic and electronic structures of composite materials is a powerful research tool of modern materials science [1-4]. When the surfaces of the components of heterostructural composite materials of different chemical compositions interact, the atoms of the components may mutually diffuse to a certain depth of their volumes. As a result, interface (interphases) layers are formed - transitional regions with unique physical properties, where atoms of both components of the material are present. The physical characteristics of such interface layers are very difficult to predict using only general ideas about atoms, ions or molecules interactions. However, the mutual diffusion of component atoms can be effectively modeled in calculations using the molecular dynamics (MD) methods. Further application of the electronic structure calculation methods to the obtained atomic structures (when coordinates of atoms optimized in MD approach are input parameters of ES calculations) allows to calculate the most important micro- and macro-characteristics of the interface layers. Such characteristics can be, in particular, the energy and spatial electronic structures, optical constants, spectra of optical absorption, electronic conductivity and others.

The report presents results of theoretical and computational studies of the atomic and electronic structures of interfaces of composites of different types using computational programs of Materials Studio 2019 software package [5]. Two types of composites were considered: a) KBi(MoO4)2 crystal - phosphate-molybdate glass of K2O-P2O5-MoO3-Bi2O3 system; b) K2Bi(PO4)(WO4) crystal - phosphate-tungstate-vanadate glass of K2O-P2O5-WO3-VO3 system. The atomic structures of interface layers of composites were calculated by MD methods implemented in Amorphous Cell and Forcite programs. The calculations were performed for ~30x30x45 Å three-dimensional periodic cells, which contained 300-500 atoms of composites. The electronic structure calculations were performed in the DFT approximation using the band-periodic plane wave pseudopotential method CASTEP, for which the cells of smaller size were used.

Obtained computational results are compared with experimental data on optical and luminescence spectroscopy of pure and Eu-doped samples of glass-ceramic composite materials. Relationships between atomic and electronic structures of interface (interphases) layers and optical characteristics of studied composites were analyzed. The possibility of "engineering" the optical properties of a number of novel composite materials is discussed.

ACKNOWLEDGMENTS

The calculations were performed using Bem supercomputer of Wroclaw Center for Networking and Supercomputing (grant no. 488).

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Study of Magnetic and Optical Properties of Mn_2CO_2 MXene

Jiri Kalmar*, Frantisek Karlicky
University of Ostrava (Czech Republic)

* kalmar.jiri@gmail.com

Abstract ID # TM -645

We have recently shown that Mn-based MXenes are promising for (opto)electronic applications and that their properties are strongly influenced by the intrinsic magnetic state[1]. Further, unusual magnetic properties make the Mn_2CF_2 MXene an optimal material for applications in spintronics[2]. We present here a thorough study of magnetism in Mn_2CO_2 MXene using larger magnetic supercells. We show that different structural and spin isomers are energetically very close with total energy differences reaching up to 0.01 eV. The electronic properties in presented isomers vary significantly, with the band gap ranging from 0.7 eV to isomers with metallic behavior. Our predictions, using standard generalized gradient approximation (GGA) to density functional theory (DFT), were also extended using selected meta-GGA density functionals. Finally, we investigate the optical absorbance properties of Mn_2CO_2 by the GW many-body method and Bethe-Salpeter equation which show that Mn_2CO_2 has an excellent absorbance in the full visible region. Together with the possibility of antiferro-ferromagnetic switching, this makes Mn_2CO_2 a very promising photovoltaic material.

ACKNOWLEDGMENTS

This work was supported by the Czech Science Foundation (21-28709S) and the University of Ostrava (SGS06/PrF/2023).

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Proximity Effects In Graphene Van Der Waals Heterostructures

Martin Gmitra[1, 2 *]
[1] *Institute of Physics, Pavol Jozef Šafárik University in Košice (Slovakia)*
[2] *Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences (Slovakia)*

* martin.gmitra@upjs.sk

Abstract ID # TM -668

Layered van der Waals heterostructures provide a versatile platform for great tunability of electronic properties via proximity effects. Proximitized spin-orbit coupling, exchange interaction, and superconductivity properties in materials that intrinsically lack these properties are of great interest for future nanoelectronics [1,2]. In this talk, we present proximity-induced spin-orbit coupling and exchange interaction in graphene on semiconducting 1H-WSe2 and metallic 1T-TaS2 transition metal dichalcogenides. We use first-principles calculations based on density functional theory and tight-binding modeling of the proximity effects on graphene electronic states. Specifically, we discuss spin patterns in graphene electronic states modified by the charge density wave and ferromagnetism in 1T-TaS2 [3], and their relevance for the generation of spin current and spin-orbit torque. Transition metal iodides encapsulated in graphene [4] represent recently discovered stable structures that provide systems with a novel interplay of proximity-induced spin-orbit coupling and electric polarization.

ACKNOWLEDGMENTS

This work was supported by the Slovak Academy of Sciences project IMPULZ IM-2021-42 and project FLAG ERA JTC 2021 2DSOTECH, Slovak Research and Development Agency provided under Contract No. APVV-SK-CZ-RD-21-0114 and by the Ministry of Education, Science, Research and Sport of the Slovak Republic provided under Grant No. VEGA 1/0105/20.

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Semiconducting MXenes: What We Can Learn About Excitons, Electronic, and Optical Properties From Many-Body Methods

Frantisek Karlicky *
University of Ostrava (Czech Republic)

* frantisek.karlicky@osu.cz

Abstract ID # TM -677

The optical properties of two-dimensional (2D) materials are accurately described by many-body methods, including specifically pronounced electron-electron and electron-hole effects. We used both accurate GW and Bethe-Salpeter equation calculations (computationally demanding and applicable on small computational cells only [1]) and time-dependent density functional theory (TD-DFT) based on specific screened hybrid density functional (an approach that effectively accounts for all important physical effects including excitons [2]) to investigate the optical and excitonic properties of two-dimensional transition metal carbides, MXenes. We determined reliable optical gaps, optical absorbance spectra, and exciton features for a set of semiconducting MXenes containing 3d or 4d metals and -O, -F, -OH, or -Cl termination groups [1,3,4]. Selected Ti-, Mn-, and Mo- based semiconducting carbides showed high monolayer absorbance of 10 - 20% in the 1 - 3 eV energy range, i.e., materials well absorbed solar radiation, including visible (VIS) light. Some Sc-, Cr-, and Mn-based carbides have an optical gap in the energy region of visible (VIS) light. We also analyzed the excitons in considered MXenes and found that the first bright excitons of Sc-, Ti-, and Mo-based MXenes are strongly localized in k-space while the corresponding excitons of Cr- and Mn-based systems are delocalized [3]. Moreover, oxygen-terminated Ti2C undergoes semiconductor-to-metal transition by the creation of a single Ti-vacancy and by compression strain [5]. Finally, we discover MXene candidates to unusual exciton insulator character [4].

ACKNOWLEDGMENTS

This work was supported by the Czech Science Foundation (21-28709S).

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Periodic Intermittent Mode of Ice Surface Softening During Friction at Deformational Defect of Ice Shear Modulus

Alexei Khomenko[1 *], Roman Chernushchenko[1], Oleksandr Goncharov[1, 2], Kateryna Khomenko[1], Yaroslava Khyzhnya[1], Iryna Shuda[1]
[1] *Sumy State University (Ukraine)*
[2] *Institute of Materials Science, Slovak University of Technology in Bratislava, Trnava (Slovakia)*

* o.khomenko@mss.sumdu.edu.ua

Abstract ID # TM -738

Ice is generally considered as an extremely slippery material because its coefficient of friction is an order of magnitude lower than that of other crystalline solids that most people meet. Historically, microscopic observations of ice surfaces have been problematic, so the processes associated with ice rubbing have been determined using an analytical approach [1, 2] or derived from the relationship between the friction force and a number of parameters used in tribological experiments [1-5]. Friction on ice has been the subject of scientific research for more than 100 years [3], and it has long been recognized that the coefficient of friction for ice strongly depends on temperature and sliding speed [1].

The relevance of the work lies in the fact that the study of the periodic mode of softening of the ice surface during friction is of fundamental importance for tribology, and can also be used to predict a decrease or increase in friction and to eliminate the negative impact of intermittent mode. The starting assumption of our approach [5] is that ice softening during friction is ensured by self-organization of the fields of strain and stress shear components, on the one hand, and the temperature, on the other. The relationship between two first components is well known, with the Kelvin-Voigt model describing its simplest case. The temperature effect is caused by critical increase in the shear modulus with decrease in the temperature: shear modulus vanishes in the water, and shear modulus is not equal to zero in the ice.

We plan to develop mathematical model that describes the periodic mode of softening of the ice surface during friction [5] on the case of deformational defect of ice shear modulus. This case corresponds to formation of premelted film with thickness about 10 nm by mechanism of first-order phase transition. Such film is very affected by noise due to small thickness. The second-order differential equations will be derived describing damped harmonic oscillations for boundary relations between the shear strain, stresses, and temperature relaxation times. In all cases, phase portraits and time series of friction force will be constructed. We will show that white noise influence leads to an undamped oscillation mode corresponding to a periodic intermittent (stick–slip) regime of friction that is basically responsible for destruction of rubbing parts. The conditions in which the periodic intermittent regime is manifested most clearly will be determined, as well as parameters for which this mode does not set in the entire range of the friction surface temperature.

ACKNOWLEDGMENTS

The work is done due to support of priority areas of scientific research and scientific and technical (experimental) developments by Ministry of Education and Science of Ukraine (additional agreement No. BF/25-2021).

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Spin Production in Helical Molecular Wires

Richard Korytár *
Charles University, Faculty of Mathematics and Physics, V Holešovičkách 2, 180 00 Prague 8, Czech Republic (Czech Republic)

* korytar@karlov.mff.cuni.cz

Abstract ID #TM-744

Various spin-selected phenomena have been recently reported for helical molecular wires (for example, the DNA). The explanation of these phenomena is still lacking [1,2]. I will present a theoretical analysis of spin currents in non-magnetic molecular junctions. First, constraints based on time-reversal invariance will be summarized. Second, I will present results based on Landauer formalism and a simple model Hamiltonian [3]. Possible experimental detection setups will be discussed.

ACKNOWLEDGMENTS

Financial support was provided by the the Czech Science foundation (project no. 22-22419S).

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The Study of ZrO_2 Materials With Different Crystalline Structure by Means of Infrared Reflection Spectroscopy

Oleksandr Melnichuk[1] *, Nadiia Korsunska[2], Yuliia Polishchuk[2], Lyudmyla Melnichuk[1], Larysa Khomenkova[2, 3]

[1] *Mykola Gogol State University of Nizhyn, 2 Hrafska str., Nizhyn 16600, Ukraine (Ukraine)*
[2] *V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine (Ukraine)*
[3] *National university "Kyiv-Mohyla academy" (Ukraine)*

* mov310310@gmail.com

Abstract ID #TM-772

Zirconia-based materials offer different applications, i.e. for microelectronics, oxygen sensors, dosimeters, fuel cells, catalysts, biological labeling etc. For most of these applications, either powder-like or ceramic-like materials are used.

To get insight on crystalline structure of zirconia-based grains (type of crystal lattice, presence of prolonged defects, etc.), the electron microscopy is used. However, being destructive method, it meets also some difficulties because of dielectric nature of ZrO2-based materials that causes charging effects.

In this work, we demonstrate the utility of infrared (IR) reflection spectroscopy for identification of crystalline structure of ZrO2-based powders and ceramics. These latter can be studied by means of specular and/or diffuse infrared Fourier transform spectroscopy.

For ZrO2 materials with different crystalline phases, the experimental spectra were recorded and their theoretical modelling was performed. This latter was based on the frequency dependence of the dielectric permittivity given by the well-known Helmholtz – Kettler formula $\varepsilon(\nu) = \varepsilon_\infty + \varepsilon_f$ [1,2].

For the cubic ZrO2 phase, a single-oscillator model was used [3], while for tetragonal and monoclinic phases – five [4] and seven [5] oscillators were considered, respectively. The spectra were simulated using the Kramers–Kronig ratio. For each case, the values of high-frequency dielectric permittivity ε_∞ were extracted from experimental IR reflection spectra whereas the static dielectric constant ε_0 was determined using the Lydden – Sachs – Teller ratio. The frequencies of transversal and longitudinal optical phonons νT and νL and corresponding damping coefficients γfL and γfT for each ZrO2 crystalline phase were determined. The obtained data were compared with those reported elsewhere for ZrO2 with different crystalline structure.

It turned out that the theoretical spectra of different ZrO2 phases showed the minimum of reflection intensity close to the high-frequency edge of the "residual rays" spectral range. The position of this minimum is the specific feature of each crystalline phase. For instance, it was centered near 700-720 cm-1 for cubic ZrO2, 790-800 cm-1 for tetragonal ZrO2 and 820-840 cm-1 for monoclinic ZrO2. Besides, the variation of phonon damping coefficients γfL and γfT effects slightly the spectral position of this minimum. Thus, the position of the high-frequency IR reflection minimum can be used to distinguish the type of crystalline structure. The experimental data obtained for ZrO2 samples with different crystalline structure confirmed this statement.

In this work the application of developed approach for the characterization of doped ZrO2 powders will be also discussed to show the utility of IR spectroscopy for express structural characterization of different polycrystalline materials.

ACKNOWLEDGMENTS

This work was supported by the National Research Fund of Ukraine from the state budget, project 2020.02/0380 "Structural transformations and nonequilibrium electronic processes in broadband oxides and their solid solutions."

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Martensite Transformations in Nanostructured ZrO_2 Films Formed on Zr-Based Alloys During Oxidation

Dmitrii Kharchenko[1], Vasyl Kharchenko[1], Olha Shchokotova[1 *], Lu Wu[2], Tianyuan Xin[2], Rongjian Pan[2]
[1] *Institute of Applied Physics National Academy of Sciences of Ukraine (Ukraine)*
[2] *The First Sub-Institute Nuclear Power Institute of China (China)*

* shchokotova.o@gmail.com

Abstract ID #TM-774

In our study, we focused on investigating the martensitic phase transformation from the tetragonal to monoclinic phase in Zirconia (ZrO2) films during the oxidation process of Zirconium alloys, specifically Zircaloy-4, ZIRLO, and Zr-1Nb. Our approach involved utilizing thermodynamic principles and considering the grain size distribution of the material.Through our analysis, we determined that the critical grain size, which governs the stability of the tetragonal phase near the oxide-metal interface, is found to be up to 20 nm, although this value may vary depending on the specific material being studied. By considering the mechanical equilibrium conditions, specifically the equivalence of in-plane stress between the metal substrate and the difference in strain resulting from oxidation expansion and compressive stress in the oxide, we discovered that both the critical grain size and the fraction of the tetragonal phase decrease with increasing distance from the oxide-metal interface.This finding provides an explanation for the non-uniform distribution of the tetragonal phase as we move away from the oxide-metal interface. Additionally, we observed that the transformation of nanometer-sized grains of the tetragonal phase can be triggered by thermal fluctuations. We noted a significant decrease in the critical grain size occurring at the fragmentation onset, which is equal to 1.27 μm. Our findings were further validated through experimental observations, confirming the accuracy of our results. Overall, our study provides insights into the martensitic phase transformation in Zirconia films during the oxidation process of Zirconium alloys, shedding light on the critical factors influencing the stability and distribution of the tetragonal phase within the material.

Spintronics With 2D Materials

Jaroslav Fabian *
Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany (Germany)

* jaroslav.fabian@ur.de

Abstract ID #TM- 810

The advent of 2D materials has revolutionized solid state physics and solid-state-based technologies. The principal driving force for the expanding exploration of the 2D realm is the highly efficient control of the physical---mechanical, electrical, optical, magnetic and spin---properties of atom-thick monolayers and their heterostructures exhibiting relatively weak but impactful van der Waals interactions. Spintronics, which aims at actively exploiting the spin of conduction electrons to introduce novel device concepts such as field-effect spin transistors, tunneling junctions based on magnetoresistance, spin-charge conversion, or spin torques, has made significant strides since the first spin injection experiments in graphene. Indeed, the fundamental aspects of the spin physics in monolayers are rather firmly established [1]. The next generation of 2D spintronics, what is the current focus of world-wide research, is based on van der Waals heterostructures, which offer tailor-made design platforms for designing novel spintronics phenomena [2]. The main mechanism by which the electron spin properties are tuned in heterostructures is the proximity effect. For example, we can design a synthetic magnetic graphene by stacking it with a 2D ferromagnetic semiconductor. More than that, the effective magnetic properties of the itinerant electrons in graphene can be tuned by gating, straining, stacking, and even twisting of such a heterostructure [3]. Similar tailor-made properties are exhibited by graphene stacked with 2D transitional-metal dichalcogenides [2], in which case graphene electrons acquire strong spin-orbit coupling. Combining ferromagnets and strong spin-orbit materials results in so exsotronic structures, with on-demand swappable spin interactions provided by gating or doping.

In this talk I will review the current stage 2D spintronics and the directions in which the research in this field is moving, from fundamentals of proximity phenomena to potential applications involving spin-charge conversion and spin-orbit torques.

ACKNOWLEDGMENTS

DFG SFB 1277, DFG SPP2244, FLAGERA 2DSOTECH, EU Graphene Flagship.

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Time Crystals Using Topological States?

David Carroll[1 *], Kamil Burak Ucer[1], Vojislav Krstic[2]
[1] *Department of Physics, Wake Forest University (United States)*
[2] *Department of Physics, FAU Erlangen (Germany)*

* carroldl@wfu.edu

Abstract ID #TM-832

In this talk I will present evidence of robust Floquet states in 2D chalcogenide nanoplates. Nanoplates of BiSe are grown and characterized using MFM, and transport They show the existence of perimeter spin states as suggested by the system's topology. The circulation of these perimeter states can be used to provide the basis of an underlying time crystal state . Using polarized subbandgap pulsed light, the spin circulation state is placed into an out-of-plane dispersive state. This state is then accumulated (MBA) using a second pulse polarized light. The technique follows a pulse sequence similar to that of other spin echo systems and the magnetization in our case is measured using the magneto-optic Kerr effect. The result is a robust beat frequency that is dependent on field strength, but not on pulse sequence timing. By varying pulse width, and field strength a standard J - epsilon phase diagram can be made for this system, showing the features of the time crystal.

Engineering the Structure and Properties of 2D Materials by Defect Creation and Intercalation

Arkady Krasheninnikov[1, 2] *
[1] *Helmholtz-Zentrum Dresden-Rossendorf e.V. (Germany)*
[2] *Aalto University (Finland)*

* a.krasheninnikov@hzdr.de

Abstract ID #TM-844

Following isolation of graphene, many other 2D systems, e.g., single sheets of transition metal dichalcogenides (TMDs) have been manufactured. All these materials contain defects and impurities, which may govern their electronic and optical properties. Moreover, defects can intentionally be introduced using beams of energetic particles – ions and electrons. Formation of defects may also give rise to phase transformations in these materials and/or tune their properties. All of these calls upon the studies on defects and mechanisms of their formation under irradiation. In my talk, I will present the results of our recent theoretical studies [1-4] of point and line defects (such as mirror twin boundaries) in 2D TMDs obtained in close collaboration with several experimental groups. I will further discuss how new 2D phases of materials can be created upon atom intercalation between graphene sheets and address the role of defects in this process [5].

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Modeling of Ti_2CO_2 QDs: Influence of Edge Functionalization and Size On Their Properties

Barbora Venosova *, *Frantisek Karlicky*
University of Ostrava (Czech Republic)

* barbora.venosova@osu.cz

Abstract ID #TM-856

In the last six years, interest in MXene-based quantum dots (MXQDs) has significantly grown. The quantum confinement effect present in QDs can significantly improve properties such as higher chemical stability and better electronic and optical properties compared to their 2D counterparts.[1] However, there is a lack of information on the structure of MXQDs, in particular the egde-functionalization and its correlation with electronic and magnetic properties. In this study we present theoretical results of density-functional analysis of Ti2CO2 QDs in which the influence of both the QDs size and edge functionalization has been studied. Calculations in different spin states were performed using the wB97XD functional together with 6-31G(d,p) basis sets. Oxygen edge funtionalization is found to be the most stable type of termination for Ti2CO2 QDs. The energy gap decreases with increasing lateral size and it was found that it can be further tuned through the modification of the functionaliziation groups. In addition we found that Ti2CO2 MXQDs of certain sizes can exhibit magnetic properties.

ACKNOWLEDGMENTS

Financial support by Czech Science Foundation (21-28709S) is gratefully acknowledged. The computations were performed at IT4Innovations National Supercomputing Center through the e-INFRA CZ (ID:90140).

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A Study On the Early Shear Deformation of Metallic Glass Using Graph Neural Network

Eunsung Jekal *
J.K.Laboratory, Republic of Korea (Republic of Korea)

* everjekal@gmail.com

Abstract ID #TM-878

Plastic deformation of metal glass that shows no long-range structural order is carried out by shear transformation of a local group of atoms called the shear transformation zone (STZ). Although significant efforts have recently been made to predict shear transformations with initial atomic properties using machine learning, studies exploring the problem of selecting appropriate predictive metrics are insufficient. Therefore, we train graph neural networks that predict initially activated STZs and evaluate their predictive power using various metrics that process imbalanced datasets. From this method, we reveal that the prediction performance is greatly changed by the threshold of the initial activated STZ due to the change in the degree of class imbalance. In addition, our work suggests that it is important to use the same threshold for this type of classification (i.e., the class ratio) and to evaluate predictive performance globally based on various metrics for fair evaluation of machine learning models adopted in different studies.

ACKNOWLEDGMENTS

This work was supported by the Material Research Council (grant number: 2023-2121).

The authors thank Dr. Mark Horstemeyer for his assistance with molecular dynamics simulation.

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TRACK 13

“INTERDISCIPLINARY & MISCELLANEOUS TOPICS”

Synthesis and Identification of Fullerene-24 Adducts with Transition Metals and Lanthanides (by the Example of Zn, Co, and La)

Botogoz Shaimordanova, Josulan Shaimardanov, Natalia Kulenova *, Marjan Sadenov, Ludmila Shushkevich, Nikolay Charykov, Victor Keskinov, Alexander Blokhin

D. Serikbaev East Kazakhstan Technical University (Kazakhstan)

* 3007kulenova53@gmail.com

Abstract ID #IMT-0478

This work deals with the synthesis and identification of nanopreparations with a set of useful functions based on fullerenes. Fullerene is an allotropic modification of carbon, and its derivatives are almost insoluble in aqueous solutions. Therefore, their widespread use could be more problematic. In this regard, creating various water-soluble derivatives of fullerenes - fullerenols, which are already widely used in various industries, is relevant. A number of researchers found that fullerenols have antibacterial and antiviral activity, as well as antioxidant properties. The antioxidant activity of fullerenols demonstrates the possibility of using these nanomaterials in crop production to improve the productivity and stability of crops. For the synthesis of water-soluble fullerenols, the most available fullerenol-24 was used. As a result, gram quantities of fullerenol-24 adducts were synthesized. The obtained adducts were identified by infrared, electron spectroscopy, high-performance liquid chromatography; mass spectrometry; and X-ray fluorescence elemental analysis. Further, the effect of the synthesized carbon-containing nanopreparations on the yield of spring barley under field conditions was evaluated. Treatment of spring barley crops with fullerenol-24 adducts was carried out twice in the phase of vegetation: tillering – the emergence of the tube. A positive effect of the studied nanopreparations on the yield of spring barley was noted. The yield increase in the treatment of experimental plots compared to the control sample was 10 - 35 % depending on the type of soil and the specific type of metal adduct.

ACKNOWLEDGMENTS

This research was supported by Project IRN BR10965186 "Development and implementation of geo-information support for "smart" agriculture to improve the management of the agro-industrial complex", funded by the Science Committee of The Ministry of Education and Science of the Republic of Kazakhstan.

Ionome Mapping and Targeted Amino Acid Metabolome Profiling of Pinto bean (Phaseolus vulgaris L.) Seeds

Imbibed with Phytoengineered Nano-zincite Guided by Molecular Dynamics Computational Simulation

Karen Jacqueline Cloete Cloete[1 *], Nandipha Botha[1], Ziga Smit[2], Kristina Isaković[3], Mahmood Akbari[4], Razieh Morad[4], Malik Maaza[1]

[1] *University of South Africa (South Africa)*
[2] *Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia (Slovenia)*
[3] *Jožef Stefan Institute, Jamova 39, SI-1001 Ljubljana, Slovenia (Serbia)*
[4] *UNESCO-UNISA Africa Chair in Nanosciences & Nanotechnology Laboratories, College of Graduate Studies, University of South Africa, Muckleneuk Ridge, PO Box 392, Pretoria, 0003, South Africa (South Africa)*
* kabouter cloete@gmail.com

Abstract ID #IMT-0488

Nanofertilizers present as a revolutionary technology to increase plant nutrient use efficiency during a time of climate change and the augmented use of traditional fertilizers which may lead to poor soil quality [1]. Albeit there has been an increased interest in the application of Zn-based nanofertilizers as a micronutrient, far less investigations have focused on the utility of green synthesized Zn-based nanofertilzers [2]. Furthermore, most studies have focused on the application of nanofertilizers as a plant growth promoting agent applied via the foliar or soil route [3], with almost no studies existing focusing on the utility of Zn-based nanofertilizers as a potential biofortification agent for seeds. Here we not only show that a Zn-based nanofertilizer has the potential to significantly boost Zn content in seeds, but also its ability to boost the metabolism of specific amino acids in Pinto bean seeds, a high value cash crop. Furthermore, we explored a multidisciplinary approach by using computational modelling and ion beam accelerator techniques to show the distribution of the phytoengineered nanoparticles within specific seed morphological regions. We found that the nanofertilizer accumulates and localizes mainly in the seed coat region where it may potentially serve as an antimicrobial agent. In addition, we show that the Zn concentration in treated seeds was augmented by more than 9 times, whilst the amino acid content of all amino acids was also slightly upregulated. Our results demonstrate both fundamental aspects of nanofertilizers on the ionome and amino acid metabolism whilst also attempting to delineate the uptake and distribution of a nanofertilizer in seeds. We anticipate that our work will serve as a starting point for further fundamental and applied studies on nanofertilizer uptake and utility as a biofortification or biocontrol agent to boost the revolutionary application of nanofertilizers in agriculture.

ACKNOWLEDGMENTS

The research leading to this result has been supported by the RADIATE project under the Grant Agreement 824096 from the EU Research and Innovation programme HORIZON 2020.

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Screening of Magnetic Field by Self-Assembled Mammalian and Fungal Microtubules

Pavlo Mikheenko *

University of Oslo (Norway)

* pavlo.mikheenko@fys.uio.no

Abstract ID #IMT-0494

Microtubules are essential structural elements in living organisms, which form scaffolding of the cells and participate in transport of proteins and separation of chromosomes [1]. They are highly ordered nanotubes built of two types of tubulin proteins and filled with water [2]. It was suggested that additionally to the transport and mechanical functions, microtubules are crucial to the processing of information [3]. Moreover, this processing is considered to be quantum-mechanical [3] and even based on superconductivity [4]. Previously, screening of magnetic field, which supports superconductivity, has been observed by magnetic force microscopy in the microtubules assembled from the mammalian tubulin [5]. Here the study is extended to the fungal self-assembled microtubules. In spite of observed structural differences between the mammalian and fungal microtubules, both display full screening of magnetic field. The temporal scans reveal steady screening in the mammalian microtubules and a fluctuating screening in the fungal microtubules. The formation of links between the microtubules and their implication for the processing of information is discussed.

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Additive Manufacturing of Bioresorbable Scaffolds Based on Polycaprolactone and Composites

Yaroslav Kravchenko[1 *], Maksym Pogorielov[2, 3], Anton Taran[4], Maksym Kubakh[1], Yevhenia Husak[1]

[1] *Sumy State University (Ukraine)*
[2] *Institute of Atomic Physics and Spectroscopy, University of Latvia (Latvia)*
[3] *Biomedical Research Centre, Medical Institute, Sumy State University, Sumy (Ukraine)*
[4] *National Science Center "Kharkov Institute of Physics and Technology" (Ukraine)*
* y.kravchenko@phe.sumdu.edu.ua

Abstract ID #IMT-0504

Additive manufacturing technology has become a significant advance in tissue engineering and regenerative medicine [1,2]. One of the first 3D printing methods to become widespread was Fused Deposition Modeling (FDM). This extrusion-based 3D printing technology is still the simplest and most affordable. In this technology, thermoplastic filaments are used as the printing material, they are liquefied and resolidified in the desired configuration. However, the application of this technology to bioprinting needed improvement and led to the development of printheads connected to a melting bin. In such printheads, the material can be in the form of granules and a mixture of powders. One of the promising polymers for which FDM printing is available is polycaprolactone (PCL) [3,4]. Polycaprolactone is a biodegradable polyester with a low melting point (59-64 degrees). It is a polymer of ε-caprolactone.

One of the biggest advantages of using polycaprolactone is its bioresorption/biodegradability. Implants made from this material can be decomposed in the body 1-3 years after implantation without harming the body [5]. A potential area for the application of polycaprolactone is the manufacture of implants and appropriate scaffolds by 3D printing for the restoration of bone and cartilage tissue, partially lost limbs and cosmetic surgeries. The advantage of 3D printing is the ability to provide an individual approach and high accuracy of passportization.

The printed scaffold has satisfactory mechanical strength. Bioresorption studies have been carried out. Several parts of the scaffold were separated and transferred to a solution of simulated human body fluid (SBF). The weight of the PCL fragments of the scaffold was 0.596 and 0.613 g, respectively. Samples were weighed every 7 days to determine weight loss. The results of the experiment indicate that in 200 days the total weight loss of the scaffold PCL fragments reaches ~1.3%. Further research will be aimed at creating nanocomposites for scaffolds in order to reduce the time of PCL bioresorption, increase biocompatibility, and stimulate osteoinductivity without losing the mechanical stability of scaffolds. In general, the development of additive manufacturing technologies is an important step in the development of medicine and biotechnology.

ACKNOWLEDGMENTS

Ya.O. Kravchenko is grateful to the Ministry of Education and Science of Ukraine for financial support (Project No. 0121U100472 and 123U100111) and the partial financial support from NCN OPUS project 2020/37/B/ST5/00576

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Expanded Graphite – Carbon Nanotubes Nanocomposite Materials

Kateryna Ivanenko[1 *], Dongxing Wang[2], Evgeny Demianenko[3], Yuliia Grebel'na[4], Mykola Tymofiiovych Kartel[3], Yurii Ivanovych Sementsov[5, 6]

[1] *Institute of Macromolecular Chemistry of National Academy of Sciences of Ukraine (Ukraine)*
[2] *Ningbo University of Technology (China)*
[3] *Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine (Ukraine)*
[4] *TMSpetsmash Ltd (Ukraine)*
[5] *Ningbo University of Technology, No 55-155 Cui Bai Road, Ningbo, 315211 (China)*
[6] *Ningbo Sino-Ukrainian New Materials Industrial Technologies Institute, Kechuang building, N777 Zhongguan road, Ningbo, 315211 (China)*

* k_ivanenko@i.ua

Abstract ID #IMT-0512

Natural graphite and materials with a graphite-like structure have the maximum possible thermal stability in a non-oxidizing environment. Therefore, when creating sp^2-hybridized carbon-carbon composite materials (CCCM) with a binder, it determines the thermodynamic characteristics of the material and the temperature range of operation. Thus, obtaining CCCM without a binder has always been and remains an urgent task. The only way to obtain solid material from natural graphite is the thermochemical modification of the surface of its particles, the so-called expanded graphite (EG) technology, which is used to produce EG and sealing materials from it. Molded EG is an elastic-plastic material that deforms under pressure and increases its bulk density, while it has a certain interval of elastic deformation at a constant density. It is this interval that determines the service life of the seal, due to material removal in the friction nodes (rod, shaft). To increase the elastic component, that is, to increase the life of the seal, we add carbon nanotubes (CNTs) - a uniquely elastic material. Here, we show the method of obtaining the EG-CNTs nanocomposite, give its structural and mechanical characteristics important for application, and, based on quantum chemical calculations, propose a mechanism for the formation of a chemical bond between oxidized graphene-like planes. Synthesis of EG-CNTs without binders consists in simultaneous deagglomeration of CNTs and intercalation of natural graphite. This procedure was carried out in two variants: electrochemical (anodic) oxidation and chemical oxidation. Graphite oxidized to the first stage (blue) was hydrolyzed, washed to neutral pH, dried and heat-treated at a temperature of ~ 1000°C in a gas horizontal industrial furnace. The resulting EG powder was rolled on horizontal rolls. X-ray photoelectron spectroscopy was used to determine the amount of oxygen and the type of oxygen-containing groups on the surface of EG and CNTs and the dependence on the amount of electricity passed during anodic oxidation. The energy effects of the interaction of partially oxidized graphene-like planes with each other and their dependence on the nature of the oxygen-containing functional groups present in them and on the dimensions of the graphene-like planes themselves were clarified by quantum chemistry methods. It was established that the most thermodynamically probable is the reaction between the hydroxyl and aldehyde groups of two interacting graphene-like planes, regardless of their sizes. Such materials are extremely promising for increasing reliability when used as mechanical seals of power equipment.

Formation of Nanostructures in the Weld Nugget Zone in Friction Stir Welding of Mg-Al Alloys

Valery Kostin[1, 2 *], Julia Khokhlova[1], Maksym Khokhlov[1], Alexey Makhnenko[1], Oleksandr Puzrin[1]

[1] *E.O. Paton Electric Welding Institute of NAS of Ukraine (Ukraine)*
[2] *Kyiv Academic University (Ukraine)*

* valerykkos@gmail.com

Abstract ID #IMT-0518

The development of solid-phase welding technologies for thin magnesium alloys MA2-1 is an actual task. The experience of obtaining high-quality butt-welded joints from sheets of magnesium alloy 2 mm thick at a constant cylindrical tool rotation frequency of 1420 rpm and various linear welding speeds - 8 m/h, 16 m/h, and 25 m/h is described. The macro- and microstructure of welds, physical and mechanical properties are studied, and it is shown that in the area under the nugget, a local zone with nanograins and primary strengthening phase of $Mg_{17}Al_{12}$ that retained in the alloy after deformation and welding. It was established that the γ-phase $Mg_{17}Al_{12}$ has the ability to be enriched with zinc and additionally with aluminum, forming an intermetallic phase $Mg_{17}(Al,Zn)_{12}$, which is dispersed during the welding process to nanoscale. Hardness and Young's modulus increased a 2-3 times at the nugget.

The TMAZ on the retreating side of the metal flow has a very contrasting plastically deformed texture. Hardening forms as a result of a few thermodynamic processes. This is due to the double pressing from above by the tool to the lower support and the rigid reaction of the lower support, and the plastic flow of the metal at a temperature close to the melting temperature of the magnesium alloy, at which the HAZ recrystallizes. An optimal union of Mg-alloy hardness and thickness and FSW pin geometry in the experiment allowed for obtaining satisfying joints.

The large inhomogeneity of the texture of the welded joint zones along the side of the FSW tool retreating (RS) in the form of a solid line of deformed grains and the inhomogeneity of the values of hardness and Young's modulus, create an elastic-deformed state of the welded joint, and this provides the traditional statistics of cracks along this line in tensile strength tests, therefore, an additional heat treatment is usually recommended, during which the hardness can be normalized by about 10%.

Obtained similar and high-quality texture of all joints of magnesium alloy sheets depends not so much on the linear speed of welding but is the result of an effective combination of the plasticity of the magnesium alloy of the Mg-Al system and the geometry of the tool, which is the most influential parameter of FSW.

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Increasing of the Photon-Magnon Coupling Strength in a System of Coupled Microwave Resonators with a Magnetic Sample

Sergey Yu Polevoy *

O.Ya. Usikov Institute for Radiophysics and Electronics NAS of Ukraine (Ukraine)

* polevoy.sergey@gmail.com

Abstract ID #IMT-0538

One of the important tasks in the field of quantum information technologies is the development of quantum converters of electromagnetic radiation from the microwave to the optical range. These converters can be used to transfer information between superconducting qubits over a considerable distance while maintaining quantum coherence [1]. Such converters can be built on the basis of a hybrid system consisting of a magnetic sample under ferromagnetic resonance (FMR) conditions and strongly coupled with microwave resonator. The strong photon-magnon coupling between resonators is a key parameter in such a system. Therefore, the purpose of this work is to increase the coupling strength between the resonator and the spin system of a magnetic sample. One way to increase the photon-magnon coupling is to increase the quality factor of the microwave resonator [2]. Thus, the systems of resonators, which support the so-called "trapped" modes with increased quality factor, are often used. Examples of such resonators are the double split-ring resonator (SRR) [3] and the double ring resonator [4]. It is known that the fields of such resonators at the frequency of the "trapped" mode are concentrated near the resonators surface. To increase the photon-magnon coupling strength and cooperativity, we propose to place a magnetic sample just in this area.

To analyze the quality factor of the resonator modes, a modified model of forced oscillations of two oscillators system was proposed, which is based on the model of two inductively coupled circuits. The modification of such model consists in the fact that the coupling coefficient between the resonators is complex. For the microwave range, this may mean taking into account the time delay in the influence of the current of one resonator to another resonator due to the non-zero distance between the resonators. It was shown that for a certain phase shift in the coupling coefficient between the resonators, there is a sharp increase in the amplitude and quality factor of forced oscillations. This theoretical conclusion is confirmed by numerical simulation of a system of double split-ring resonators with a "trapped" mode observed at a certain frequency. For such mode, the magnetic field distribution is concentrated mainly in the area between the split-rings. When the yttrium iron garnet magnetic film is placed in this area, it was found that the photon-magnon coupling strength and cooperativity increases at the "trapped" mode frequency compared to the mode observed for a single SRR. This should be explained by the large Q-factor of the double SRR at the frequency of the "trapped" mode.

Thus, for a system of double split-ring resonator with a magnetic film, a large value of photon-magnon strength and cooperativity was achieved numerically at the frequency of the high-quality "trapped" mode.

ACKNOWLEDGMENTS

This work is supported by NATO Science for Peace and Security Program, NATO SPS project No. G5859.

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A Simple Electrochemical: Ultrasound Technique for Obtaining Biocidal Antiviral, Antibacterial and Antifungal Nanoparticles of Calcium Carbonate from the Eggshell Waste

Olga G. Bordunova[1 *], Rimma V. Dolbanosova[2], Valeriy B. Loboda[3], Yevgeniya A. Samokhina[4], Kovalenko M. Lidiia[5], Opara O. Victor[6], Chernyavska O. Tatyana[7], Andriy Stepanenko[8], Chivanov D. Vadym[9]

[1] *Dept. of Biochemistry and Biotechnology Sumy National Agrarian University (Ukraine)*
[2] *Dept. of Therapy, Pharmacology, Clinical Diagnostics and Chemistry Sumy National Agrarian University (Ukraine)*
[3] *Engineering-Technological Department Sumy National Agrarian University (Ukraine)*
[4] *Dept. of Animal Breeding and Selection and Aquatic Bioresources Sumy National Agrarian University (Ukraine)*
[5] *Department of Anatomy, Normal and Pathological Physiology Sumy National Agrarian University, Sumy (Ukraine)*
[6] *Dept. of Feed Technologies and Animal Feeding Sumy National Agrarian University Sumy (Ukraine)*
[7] *Dept. of Animal Breeding, Selection and Biotechnology Sumy National Agrarian University Sumy (Ukraine)*
[8] *Sumy State University (Ukraine)*
[9] *Dept. of Radiation Biophysics Institute of Applied Physics (IAP), NAS of Ukraine Sumy (Ukraine)*
* vadym58@gmail.com

Abstract ID #IMT-0544

Calcium carbonate nanoparticles ($CaCO_3$ NPs) have been widely used in biomedicine due to their biocompatibility and biodegradability [1]. Recently, $CaCO_3$ NPs are largely integrated with biocidal antiviral, antibacterial and antifungal agents and imaging contrast and therapeutic agents for various imaging and therapeutic approaches. The authors present work on the development of a simple electrochemical : ultrasound technique [2] for obtaining $CaCO_3$ NPs from the chick eggshells waste and other nanobiocarbonates, then the state-of-the-art progress of $CaCO_3$ NPs in treatment of the surfaces of equipment used in industrial poultry and livestock farming contaminated with pathogenic microflora was summarized. Aqueous solutions of acetic (or peracetic) acid) (0.1-10 % vol.) were used as the electrolytic liquid. The titanium anode and cathode were placed outside (anode) and inside (cathode) of the shell halves. Electrolytic liquid outside and inside the halves did not mix during electrolysis and ultrasound treatment (30 min, 70-75ºC). The eggshell undergoes destruction in an acidic medium and ultrasound treatment (22 kHz) with the formation of ultra- and nanodispersed particles $CaCO_3$ NPs. The synthesized $CaCO_3$ NPs are characterized using SEM. The diameter of the $CaCO_3$ NPs is estimated to be 97 -130.8 nm. It was shown by thermal programmed mass-spectrometry (TPD-MS) [3] method that solid-phase precipitates obtained by drying from an electrolytic liquid inside and outside the shell contain $CaCO_3$ NPs. The sample obtained at the cathode (the inner part of the shell) is distinguished by a smaller particle size. It has been shown that the structure of the TPD-MS spectrum of the carbonate part of the eggshell is a function of the level of dispersity of the components of this biocomposite. An increase in the concentration of ultrafine and micro- nano- disperse $CaCO_3$ components in the eggshell biocomposite leads to a significant change the type of the thermal desorption spectrum of CO_2, which is manifested in the appearance of additional temperature regions of desorption (peaks) and their shift to a region of lower temperatures. It has been experimentally proven that the main reason for the higher degree of dispersion of the $CaCO_3$ NPs precipitated during treatment with electricity and ultrasound on the cathode is the presence in incubation medium of specific proteins from the inner membranes and the mammillary layer of the eggshell. Protein in this case is a dispersing component, which prevents the reverse agglomeration of nanoparticles into large agglomerates. Finally, we discussed the challenges and recommendations for future studies of the electrochemical : ultrasound technique obtained $CaCO_3$ NPs as biocidal antiviral, antibacterial and antifungal substances.

ACKNOWLEDGMENTS

The work has been performed under the financial support of the Ministry of Education and Science of Ukraine (state registration number 0116U002623).

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Peculiarities of the Surface Structure of High-Speed Steel after Pulse-Plasma Treatment

Olga Kushnarova *, Olena Berdnikova, Yuriy Tyurin, Oleg Kolisnichenko, Tetyana Alekseienko, Yevhenii Titkov

E.O. Paton Electric Welding Institute of NAS of Ukraine (Ukraine)

* olgakus@meta.ua

Abstract ID #IMT-0560

The work studied the patterns of structure formation and its influence on the properties of the surface layers of high-speed steel P6M5 under different modes of pulse plasma treatment (PPT). Mode I – direct impact of the pulsed arc (the distance from the plasmatron to the sample is 60 mm); Mode II – indirect impact (distance from the plasmatron - 30 mm).

The work studied the patterns of structure formation and its influence on the properties of the surface layers of high-speed steel P6M5 under different modes of pulse plasma treatment (PPT). Mode I – direct impact of the pulsed arc (the distance from the plasmatron to the sample is 60 mm); Mode II – indirect impact (distance from the plasmatron - 30 mm).

It was established that PPT of the surface of P6M5 steel in mode II leads to dispersion by 1.5–2 times of the austenitic-martensitic structure with a 20% increase in microhardness (HV up to 9200 MPa) along the depth of the modified layer up to 40 μm from the surface. The substructure size is reduced to 120–160 nm at the density of dislocations in austenite $\rho = 4\times10^{9}$ cm^{-2} and martensite $\rho = 2\times10^{11}$ cm^{-2}. Globular shaped carbides of Me_6C type $(FeCr)_3(W, Mo)_3C$ predominantly with tungsten were found in the hardened area.

PPT in mode I leads to: melting of the surface layer up to 5 μm in depth; weakening of the metal HV = 6200 MPa to a depth of up to 40 μm; a general decrease in ρ to 10^{8}–10^{9} cm^{-2} in austenite and $\rho = 10^{9}$–10^{10} cm^{-2} in martensite. Microcracks were detected along the grain boundaries of residual austenite and carbides. Dislocation clusters are formed when the dislocation density increases to $\rho = (2–4)\times10^{10}$ cm^{-2}.

Analytical evaluations of the structural strengthening of the metal show that in the mode II the general level of strengthening of the metal of the surface layer increases by 25% to $\Sigma_{\Delta\sigma}$ = 1400–2160 MPa. The largest contribution to $\Sigma_{\Delta\sigma}$ is mainly made by the components of substructural 490–870 MPa, grain 440–640 MPa, dislocation 200–283 MPa and dispersion hardening 60–150 MPa mechanisms. This is due to the grinding of the structure, the increase in the overall dislocation density, as well as dispersion strengthening in the surface layers of steel during PPT in mode II. At the same time, the index of fracture toughness in the modified layer is 35% higher than on mode I.

PPT on the mode II leads to structural changes that provide a significant increase in the operational properties of high-speed steel P6M5.

As a result of the conducted research: the influence of technological modes of PPT on the structure of the surface layers of steel P6M5 was studied; regularities of the formation of the structure of surface layers during PPT were established, namely, the features of the thin structure by the TEM studies; analytical evaluations of strength and crack resistance were carried out; practical recommendations for the creation of surface strengthening layers of P6M5 steel using PPT have been developed.

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Antibacterial Application Of ZnO And CuO Nanoparticles In Polyelectrolyte Multilayers

Nives Matijaković Mlinarić[1 *], Anamarija Zore[1], Aleksander Učakar[2], Klemen Bohinc[1]

[1] *Faculty of health sciences, University of Ljubljana (Slovenia)*
[2] *Jožef Stefan Institute, Jamova 39, SI-1001 Ljubljana, Slovenia (Slovenia)*
* matijakovicn@zf.uni-lj.si

Abstract ID #IMT-0568

Both viruses and bacteria pose a serious threat to public health. Their structural properties allow them to bind to textile (nylon, polyester, cotton), plastic and metal surfaces. To protect people from infections transmitted through textiles and surfaces, an optimal way must be found to prevent the spread of microbes. Many textiles cannot be washed at the high temperatures required to kill microbes. In addition, surfaces in hospitals, shops and buildings may not be fully disinfected, and microbes can be spread by touching the surface and continuing to transmit them. Metallic nanoparticles have been presented as a possible solution. Due to their advantageous properties such as durability, lower toxicity to human cells and high stability, metallic NPs are ideal for antibacterial [1] and antiviral [2] applications. Currently, CuO and ZnO NPs are in the focus of research because of their antimicrobial activity. As microelements in the human body, they are both biocompatible and interesting for daily use [3], [4].

Here, we have shown that CuO and ZnO nanoparticles with different size and morphology exhibit different surface properties, modify the properties of treated surfaces (textile materials, Teflon and stainless steel) and show promising antibacterial activity against Staphylococcus aureus as part of polyelectrolyte multilayers. We fabricated nanoparticles that exhibited flaky, spherical and rod-like morphology and were characterised by varying nanoparticle size and distribution. The polyelectrolyte multilayers were formed by the sequential adsorption of polyanions (PSS or alginate), polycations (polyallylamine hydrochloride) and nanoparticles to form 6 layers between which the nanoparticles were incorporated. Coatings with different concentrations of nanoparticles showed promising antibacterial activity against Staphylococcus aureus. Our results show that the size, morphology and type of surface material play an important role in the antibacterial activity and shed light on the best approach to treat surfaces for the best results in killing bacteria by ion release from polyelectrolyte multilayers. The knowledge gained from this research forms the basis for the development of new methods in which hard surfaces and textiles are treated with polyelectrolyte and nanoparticle suspensions to produce materials with antibacterial properties.

ACKNOWLEDGMENTS

The authors acknowledge the financial support from ARRS project no. N1-0264

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Bactericidal Properties Dependent with the Dimension of Nanopillars and Elastic Modulus on Polymeric Nanopillars

Ikki Shingeya*, Takeshi Ito, Tomohiro Shimizu, Shoso Shingubara

Kansai University (Japan)

* k328807@kansai-u.ac.jp

Abstract ID #IMT-0579

The structure with numerous nanoscale pillars, called "nanopillar", is found on the wing surface of cicadas which express antibacterial and bactericidal properties physically.[1)] Recently, the number of deaths due to the infection with antimicrobial resistant (AMR) bacteria has been increasing.[2)] The nanopillar is focused to solve this issue as a novel antimicrobial material because of the bactericidal properties against bacteria with AMR.[3)~5)] In order to apply these nanostructures to medical devices and other applications, many researchers fabricated polymeric nanopillars and studied their bactericidal properties. However, there are few reports focusing on the effect of nanopillar dimensions and elastic modulus to the bactericidal properties yet. Here, we show that smaller nanopillars or polymers with higher elastic modulus have stronger bactericidal effects against *E. coli*. We fabricated some polymeric nanopillars of different dimensions and elastic modulus by thermal nanoimprint lithography using anodized aluminum oxide as molds and tested their bactericidal properties against *E. coli*. As the results, we found that lower nanopillars showed stronger bactericidal properties for the same diameter and nanopillars with higher elastic modulus showed stronger bactericidal properties when the dimension of nanopillars were the same. These results indicate that the less the pillars bend, the more mechanical stress is applied to the cell membrane of *E. coli* at the connection between the cell and the nanopillar. Our research would help to elucidate the mechanism of mechanical bactericidal properties by nanopillars. We also hope that we will contribute the development of mechanical antimicrobial materials with polymeric nanopillars and decrease in the number of deaths caused by bacteria with AMR.

ACKNOWLEDGMENTS

We are grateful to the company that provided us with polymer films and all other those involved in our research for helpful discussions.

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Magnetite as a Versatile Material,- Application as an Electrochemical Sensor in the Determination of Sucralose and Perilartin In Drinks and as an Adsorbent of Uranium: Theoretical Description

Adrianna Biedrzycka[1 *], Volodymyr Tkach[2], Evgeny Demianenko[3], Viktoriia Paientko[1, 4], Agnieszka Gładysz-Płaska[1], Ewa Skwarek[1]

[1] *Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland (Poland)*
[2] *Chernivtsi National University (Ukraine)*
[3] *Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine (Ukraine)*
[4] *Chuiko Institute of Surface Chemistry, NAS of Ukraine (Ukraine)*
* biedrzyckaadrianna@gmail.com

Abstract ID #IMT-0588

The iron oxides deserve special attention due to their distinguished features, e.g., magnetism and pervasiveness. These oxides exist in various forms and find applications in many branches of industry. Nevertheless, most studies deal with magnetite (Fe3O4) and maghemite (Fe2O3), wherein the first one is more common. Magnetite is a mineral with metallic sheen. Its structure is composed of both Fe (II) and Fe (III) ions with a 1:2 ratio. This mixed oxide displays excellent magnetic properties and electrical conductivity. Magnetite occurs naturally in rocks and can be transformed into other forms. In turn, maghemite is built of Fe (III). This mineral is unstable in the environment and can convert into the hematite form at higher temperatures. The magnetic properties exhibited by iron oxides could be a vital factor that is crucial for any potential possible applications, e.g. in medicine, adsorption, industry. In the experiment the co-precipitation method was used to obtain iron oxide. The material was analyzed utilizing the following methods: XPS, SEM, ASAP. Moreover, the zeta potential was also measured as well as surface charge density in potentiometric titration method. In this approach the original computer program titr.v3 created by Professor Władysław Janusz was used. The experiment with uranium ions adsorption on the iron oxide was also conducted and it showed high adsorption efficiency. The concentration of uranyl ions in the equilibrium solutions was determined by the spectrophotometric method. The uranium ions binding process can be assumed as mixed. It can be concluded that the iron oxide could be a good adsorbent for uranium ions. The theoretical calculations of the adsorption of uranium ions on the iron oxide surface have been carried out [1,2]. Other interesting applications of magnetite is electrochemical sensor. Perillartine (perillaldehyde anti-aldoxime) is a natural sugar substitute, extracted from Japanese perilla (shiso) leaves. Besides of the proper perillartine, its ether derivative is also used, despite of being much less sweet than the proper perillartine (possessing the sweetness, nearly equal to that of aspartame). This oxime is bioavailable and biodegradable. It may be allergic for people allergic to shiso herb. Also, some toxic nitrogen derivatives like hydroxylamine may form during its metabolism in some people. It is important to mention that perillaldehyde aldoxyme and its derivatives are rarely used as sweeteners outside Japan, so this statement may be used in investigation of falsification of allegedly Japanese product claimed to contain the peryllartine. Thus, the development of an efficient, exact and rapid method for perillartine determination is really actual task, and the electroanalytical methods would give it a good service. In this work, the electrochemical determination of sucralose and perilartine in beverages on Fe3O4-modified electrode has been theoretically described [3].

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Nano-Sized Chitosan and Plasma-Activated Water: Improving the Microbiological and Physicochemical Properties of Vetch (Vicia sativa L.) Bean Sprouts

Olha Vasylenko[1 *], Tatyana Holovko[2], Mykola Golovko[2], Vasyl Pasichnyi[3], Nadiia Lapytska[4], Qin Xuanxuan[5], Luo Yanghe[5]

[1] *Sumy National Agrarian University (Ukraine)*
[2] *State University of Biotechnology (Ukraine)*
[3] *National University of Food Technologies (Ukraine)*
[4] *T. Shevchenko National University «Chernihiv Colehium» (Ukraine)*
[5] *Hezhou University (China)*

* vasylenko.sumy@gmail.com

Abstract ID #IMT-0601

Edible sprouts, as well as powder based on them, are common food ingredients and are widely used in various cuisines around the world. In recent decades, sprouts have gained considerable popularity due to their high nutritional value and health benefits [1]. Legume sprouts are an excellent source of nutrients, micro- and macroelements for vegetarian, children's and sports nutrition. A variety of dried chopped vegetables, press cake and grist to improve digestion are included in the human diet [2], bean sprouts are no exception. Bean sprout powder combines well with other natural food ingredients to create balanced food compositions [3]. Despite the benefits for the food industry, there are many challenges in cultivation, including contamination of beans and sprouts by foodborne pathogens and plant salt stress. Vegetable seeds and beans are a source of pathogenic microorganisms, they require a warm and moist environment for germination and growth, which is a favorable environment for the reproduction of microorganisms [4]. Because sprouts require increased attention to microbiological safety indicators, chemical, physical, biological, and combined cultivation and processing strategies have been developed to affect sprout contamination by foodborne pathogens. The quality of vegetable and bean seeds is significantly affected by soil salinity, which causes a decrease in plant growth, both due to ion toxicity and osmotic stress, which is a challenge for the agricultural industry [5]. To solve these problems, nano-sized chitosan and plasma-activated water are used at the stage of germination and cultivation. Nano-sized chitosan significantly reduces the effect of salt stress on the germination of beans, and plasma-activated water reduces the number of microbes, both on the beans and on the sprouts themselves.

Standard raw materials for growing sprouts are alfalfa, broccoli, mung bean, and radish sprouts. The research uses vetch (Vicia sativa L.) beans, which have small beans (45-60 g per 1000 seeds) and are suitable for replacing standard raw materials. Nanochitosan has played an important role as a potential priming agent used in Solid Matrix Priming on saline soils. Nanochitosan has been shown to mitigate oxidative stress caused by salinity and the presence of large amounts of protein. The results of this study showed that cleaning with plasma-activated water can effectively deactivate bacteria, yeast, and mold on vetch bean sprouts in a time-dependent manner. The combination of plasma-activated water and priming agents (nanochitosan) showed an effective result, which increased the physicochemical parameters of vetch (Vicia sativa L.) bean sprouts and reduced the number of plasma-activated water treatments to significantly reduce microbiological activity on vetch (Vicia sativa L.) beans and sprouts.

ACKNOWLEDGMENTS

The authors would like to thank Sumy National Agrarian University for providing laboratory facilities and technical support during this research work

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Improved Surface Micromachined Sensors for Landslide Monitoring using Topology Optimization

Hossein Rostami Najafabadi[1], Thiago Martins[2], Ahmad Barari[1 *]

[1] *Ontario Tech University (Canada)*
[2] *Escola Politecnica da Universidade de Sao Paulo (Brazil)*

* ahmad.barari@uoit.ca

Abstract ID #IMT-0640

Landslides are natural disasters happening mostly after heavy rains. Each year landslide causes significant damage to infrastructure and endangers human lives in Brazil. Micromachined MEMS sensors have been widely used as a cost-effective alternative to monitor the deformation and movement of slopes to predict the occurrence of a landslide and evacuate the place. However, the performance of these sensors is limited by their structural design. Thin films deposited as the structural layer in surface micromachined accelerometers provide a light proof mass with low sensitivity and high noise density. Topology optimization is a powerful method to distribute material within a given design space to improve a desired objective while avoiding constraints. In this paper, we propose the application of topology optimization to improve the performance of a surface micromachined sensor to be used in landslide monitoring. The paper includes the structural design of MEMS accelerometers and the objective of the design to be optimized. Then, a topology optimization method is applied to improve the objective function while considering the manufacturing constraints. A similar design from the literature was used to compare with the results of topology optimization. A comparison of simulation results for the reference design and the proposed design demonstrates significant improvement of the surface micromachined sensor by increasing the sensitivity in the direction of measurements. Moreover, the optimized structure is more robust to the lateral motions. The proposed design shows the potential of using topology optimization to improve the performance of surface micromachined sensors in landslide monitoring. It can lead to the development of more accurate and reliable landslide monitoring systems.

Electrospun Nanofibers for Effective Oral Delivery of Efavirenz

Faseehuddin Ahmed Mohammed *

Talla Padmavathi College of Pharmacy, Warangal, INDIA (India)

* fasee1977@gmail.com

Abstract ID #IMT-0665

The recent past has witnessed tremendous efforts to develop new chemical entities with promising therapeutic efficacy via artificial intelligence tools. Though many of the developed drug candidates exhibited desired therapeutic responses during pharmacological screening, many could not reach the market due to poor oral bioavailability which is mostly due to poor aqueous solubility, poor intestinal permeability, or both.[1] Though solid dispersions via hot melt extrusion have evolved as a strategy for improving solubility, devitrification of the amorphous cargo limits its success. The recent past has witnessed the rise of electrospinning technology for the fabrication of nanofibers.[2] Efavirenz (EFV) is a widely prescribed antiretroviral drug grouped under Biopharmaceutical Classification System (BCS) class II exhibiting poor aqueous solubility and high intestinal permeability.[3] In this study, efavirenz-loaded polymeric nanofibers were developed using the principles of Quality by Design (QbD) for the improvement of solubility and in vitro dissolution of the loaded drug.

A response surface randomized Box-Behnken quadratic design with 17 runs was deployed for product development. Three important electrospinning variables i.e., DC voltage, flow rate, and polymer concentration, were studied at three levels. The characterization of the nanofibers was performed using scanning electron microscopy (SEM), differential scanning calorimetry (DSC), and powder X-Ray diffractometry (PXRD). Further, saturation solubility, and in vitro dissolution studies were carried out. The optimized nanofibers' diameter varied from 895 nm to 2.5 micrometers. The DSC studies suggested the existence of EFV in the amorphous state (sharp melting endotherm of EFV was absent) which was supported by PXRD studies (decreased intensities). There was a significant improvement in saturation solubility and in vitro dissolution of efavirenz from the nanofibrous samples compared to the naïve EFV sample.

ACKNOWLEDGMENTS

The work is funded by the All India Council for Technical Education (India) under Research Promotion Scheme (F.No. 80-27/FDC/RPS (Policy -1)/2019-20).

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Effect of Photoelectron Traps on X-Ray Induced Luminescence of Polycrystals Sintered from Y_2O_3 Nanopowder

Eugeniy Barannik, Sergiy Kononenko *, Oganes Kalantaryan, Vitaliy Zhurenko, Volodymyr Chishkala

V. N. Karazin Kharkiv National University (Ukraine)

* sergiy.i.kononenko@gmail.com

Abstract ID #IMT-0672

It has been shown recently, that under X-ray long-term irradiation the luminescence intensity of polycrystalline samples of yttrium oxide in the light emission band associated with self-trapped exciton pairs of electrons and holes, decreased essentially with a time. For X-rays with 50 keV photon energy, which were used in the luminescence experiments, the main mechanism of interaction of the radiation with matter is photoelectric effect. The developed quantitative model of the luminescence is based on the assumption that some of the high-energy photoelectrons can be captured by intergrain caverns as natural traps. It means that the source of high-energy primary photoelectrons can be divided into two parts, one of which describes the source power of photoelectrons which will be captured and another describes photoelectrons responsible for the formation of self-trapped excitons. The probability of nonexcitonic relaxation is directly proportional to the concentration of captured high-energy electrons. As a result, the fraction of photoelectrons involved in the exciton formation decreases as the concentration of captured electrons increases with time. According to the proposed model, the decrease over time of the fraction of electrons involved in exciton formation leads to the exponential damping of the luminescence intensity, which is in a good agreement with the experimental data. The degree of photoelectron trap influence on the decrease of the luminescence intensity with time depends on the ratio of the total volume of intergrain caverns to the total volume of the polycrystalline sample and on the projected path length of high-energy photoelectrons.

Precision Uncertainty Due to Infill in Additive Manufacturing of Small-Scale Devices

Yasaman Farahnak Majd*, Ahmad Barari

Ontario Tech University (Canada)

* yasaman.farahnakmajd@ontariotechu.net

Abstract ID #IMT-0681

Additive manufacturing (AM), or 3D printing, has become increasingly prevalent and is being widely employed as a fabrication approach across diverse sectors, including its applications in small-scale devices, where it offers advantages such as simplified fabrication processes, topologically optimized designed structures, multi-materials, customized anisotropic behaviors, and faster prototyping. Achieving high accuracy is of paramount importance in AM, as it ensures the precise fabrication of complex geometries and functional parts, especially in microscale and nanoscale devices, where even minor fabrication errors can significantly impact their performance and functionality. One of the sources of errors in additive manufacturing arises from the patterns used to fill the internal structure of the fabricated parts. This paper focuses on investigating the volumetric density percentage error in additive manufacturing processes, which quantifies the disparities between the nominal infill density and the actual infill density. The goal of this research is to optimize the parameters that affect this error, aiming to achieve the desired nominal infill density in AM parts.

Wireless Actuation and Mechanical Properties of Poly-Catecholamine Nanomembranes

Adam Krysztofik[1 *], Marta Warżajtis[1], Mikołaj Pochylski[1], Marcel Boecker[2], Tommaso Marchesi D'Alvise[2], Christopher V. Synatschke[2], Tanja Weil[2], Bartłomiej Graczykowski[1]

[1] *Faculty of Physics, Adam Mickiewicz University, ul. Uniwersytet Poznańskiego 2, 61-614 Poznań (Poland)*
[2] *Max Planck Institute for Polymer Research, 55128 Mainz (Germany)*
* adam.krysztofik@amu.edu.pl

Abstract ID #IMT-0704

The search for nature-inspired materials mimicking simple muscle contractions became an important research topic in recent years due to numerous potential applications in the field of soft-robotics, biomedicine, and tunable metamaterials. Among different strategies for the efficient conversion of energy contained in chemical or physical stimuli into macroscopic deformation, light-responsive materials appear as promising candidates to mitigate many current challenges. Foremost, light as a stimulus offers remote, spatial, and temporal control over actuation.

Here, we show that the light-to-motion conversion can be realized in various poly-catecholamines, including polydopamine, poly-levodopa, and poli-epinephrine. The free-standing, membranes contract upon illumination and spontaneously expand in dark conditions. This reversible, light-triggered dynamics results from the desorption and adsorption of water molecules. Moreover, using Brillouin Light Scattering spectroscopy, the determined values of the Young Modulus point to excellent elastic properties of the membranes and suggests their suitability for self-supporting applications. Our findings demonstrate that the poly-catecholamine membranes can be utilized as building blocks for soft, nanoscale actuators stimulated by light.

ACKNOWLEDGMENTS

The authors acknowledge financial support from the National Science Centre of Poland (NCN) through the OPUS grant 2021/41/B/ST5/03038.

Bioluminescence as an Indicator of the Effectiveness of Static Magnetic Fields Influence on Living Organisms

Olena Gromozova[1 *], Victor Martyniuk[2], Ihor Hretskyi[1], Oleksandr Artemenko[3], Victoriia Kobernyk[1], Oleksandr Kisten[1], Yuliya Tseyslyer[3]

[1] *D.K. Zabolotny Institute of Microbiology and Virology of the National Academy of Sciences of Ukraine (Ukraine)*
[2] *National Taras Shevchenko University of Kyiv (Ukraine)*
[3] *Taras Shevchenko National University of Kyiv (Ukraine)*

* gren.elen@gmail.com

Abstract ID #IMT-0746

The influence of magnetic fields on biological objects is an important problem in terms of the environment and human health. At the same time, the study of the molecular and cellular mechanisms of magnetosensitivity in the biological world is an important fundamental interdisciplinary problem. Present day, the dominant hypothesis regarding the molecular mechanisms of magnetic field reception is based on the idea that magnetic fields affect free radical processes in the active center of cryptochromes that catalyze the oxidation of flavins with the participation of free radical reactive species of oxygen [1]. Some data indicate that sufficiently weak magnetic fields can affect free radical processes [2]. There are also detailed theoretical explanations of the mechanisms of influence of magnetic fields on processes in the active center of cryptochromes [1]. Nevertheless, experimental verification of this hypothesis remains insufficient and requires the use of adequate biological test systems based on the processes of free radical oxidation of flavins.

Photobacterium phosphoreum is a highly sensitive microorganism used for bioindication of various chemical and physical effects. The molecular mechanism of bacterial bioluminescence is based on the free radical oxidation of reduced forms of flavins by the bacterial luciferase enzyme. Thus, this biological object is a convenient model for studying the effects of magnetic fields and provides new prospects for the development of new biosensor systems for assessing the biological effectiveness of electromagnetic effects.

We investigated the effect of a static magnetic field with induction in the range of 60 - 8000 μT for 96 hours on the bioluminescence intensity of *P. phosphoreum* cultured in liquid media and on the cellulose disks.The static magnetic field mainly weakly stimulated bacterial luminescence during the first two days in the range of 10-30% relative to the control values. After 1.5-2 days, at certain values of magnetic field induction, the intensity of bacterial luminescence was suppressed. Thus, the effect of the magnetic field depends on both the magnetic field induction, time of exposure, and also the state of the bacterial culture (cell density, accumulation of metabolic products, etc.). It is important to note that we observed a stimulating effect of the static magnetic field on the bioluminescence of photobacteria in the range close to the variations of the static magnetic field in reinforced concrete rooms of 60-100 μT.

ACKNOWLEDGMENTS

This research was funded by the project № 9918 "Magnetism in Ukraine Initiative".

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Investigating The Link Between Electrical Properties And Surface Terminations Of Carbon-Based Nanomaterials

Sofia Sturari[1 *], Veronica Varzi[1], Pietro Aprà[1], Adam Britel[1], Nour-Hanne Amine[1], Greta Andrini[2], Emilio Corte[1], Giulia Tomagra[3], Lorenzo Mino[4], Paolo Olivero[1], Federico Picollo[1]

[1] *Department of Physics, University of Torino (Italy)*
[2] *Department of Electronics and Telecommunications, Politecnico di Torino (Italy)*
[3] *Department of Drug and Science Technology, University of Torino (Italy)*
[4] *Chemistry Department, University of Torino (Italy)*

* sofia.sturari@unito.it

Abstract ID #IMT-0778

Among carbon-based nanomaterials, both nanodiamonds (NDs) and reduced graphene oxide (rGO) have attracted researchers' attention due to the possibility of esily tuning their features, respectively through the modification of their surface via thermal processes in controlled atmosphere and their mixing with metal oxides, such as titanium dioxide (TiO_2). NDs and rGO have been widely investigated for several different applicative contexts, including innovative sensors and biosensors, biomedical field and photocatalysis. In these kinds of applications, the characterization of electrical properties is a fundamental step toward practical uses, since it allows the understanding of the correlation between conductivity and material surface chemistry and structure. In the present work, we tested the electrical properties of NDs upon various thermal treatments in air, hydrogen and inert atmosphere [1] and rGO, obtained through different reduction processes from graphene oxide, and added to TiO_2 nanoparticles, interpreting the results in connection with the insights from infrared and Raman spectrocopies. Electrical measurements have been performed in controlled humidity conditions to consider the influence of water on conductivity. This indeed activates Grotthus mechanism-mediated conduction when hydrophilic oxygen-containing moieties are present on the surface [2]. Moreover, in hydrogen-terminated NDs water triggers the so-called transfer-doping, *i.e.*, an electron transfer from the material, causing the formation of a sub-surface hole accumulation layer, which results in p-type electrical conductivity [3]. On the other hand, the impact of water on the electrical behavior of sp^2 carbon phases, which are inherently conductive, appears to be negligible, due to their hydrophobic character. Our findings contributed to elucidating the complex combination of the different mechanisms responsible for electrical conduction in NDs and rGO materials, thus paving the way for further studies in the context of their development for a broad set of different applications and presenting, at the same time, a method, based on coupling spectroscopic tools with electrical characterization, which can be useful for future research.

ACKNOWLEDGMENTS

The work was supported by: "RESOLVE" project funded by the Italian Institute of Nuclear Physics (INFN); "BiophysiX" project funded by the CRT Foundation; "QuantDia" project funded by the Italian Ministry for Instruction, University and Research within the "FISR 2019″ program; "LasIonDef" project funded by the European Research Council under the "Marie Skłodowska-Curie Innovative Training Networks" program; "Departments of Excellence" grant (L. 232/2016) funded by the Italian Ministry of Education, University and Research (MIUR) and 20FUN02 "POLight" project, that has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme.

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The Role of Carbon Nanotubes in Improving the Interfacial and Mechanical Properties of Carbon Fiber Epoxy Laminated Composites.

Vaibhav Jain[1, 1 *], Satish Jaiswal[1], Kinshuk Dasgupta[2], Debrupa Lahiri[1]

[1] *IIT ROORKEE (India)*
[2] *Bhabha Atomic Research Centre Mumbai, India (India)*

* vjain@mt.iitr.ac.in

Abstract ID #IMT-0790

CF-EP composites are widely used due to their excellent stiffness, strength, and low specific weight properties. However, the brittleness of the epoxy matrix limits their use by reducing their fracture toughness. One solution to this problem is introducing a carbon-based nanofiller to reinforce the matrix. Carbon nanotubes (CNTs), with high ultimate strength, elastic modulus, and excellent fracture toughness, are promising nanomaterials for this purpose. In this study, a multiscale fiber-reinforced epoxy laminate composite is fabricated and evaluated for potential structural applications by incorporating CNTs to improve the mechanical properties. The composite is composed of carbon fibers, epoxy, and CNTs. The dispersion of CNTs into the epoxy is achieved using a probe sonicator, followed by impregnating reinforced epoxy into the carbon fiber using the vacuum impregnation technique. Tensile and 3-point bending tests are conducted on the fabricated samples, which show notable improvement in tensile strength and interlaminar fracture toughness. Modulus mapping is also carried out to understand the interfacial interaction between carbon fiber and reinforced epoxy, which influences the mechanical behavior of the multiscale composite. This study provides insights into the fabricated multiscale composite for potential structural applications.Interface, Carbon nanotubes, Nanocomposite, Carbon fiber

ACKNOWLEDGMENTS

Board of Research in Nuclear Sciences (BRNS), India, for funding the research through sanction no. 36(2)/14/17/2016-BRNS/36017

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Chitosan Film Surface Nanotexturing by Femtosecond Laser Treatment

Oksana Kalinkevich[1 *], Aleksei Kalinkevich[1], O. Yu. Karpenko[1], Yana Trofimenko[1], Viktoriia Holubnycha[2], Liliya Angelova[3], Viktoriia Ivchenko[4], Albena Daskalova[5]

[1] *Institute of Applied Physics, National Academy of Sciences of Ukraine (Ukraine)*
[2] *Biomedical Research Centre, Medical Institute, Sumy State University, Sumy (Ukraine)*
[3] *Institute of electronics, Bulgarian Academy of sciences (Bulgaria)*
[4] *Sumy National Agrarian University (Ukraine)*
[5] *Institute of electronics,Bulgarian Academy of sciences (Bulgaria)*

* oksana.kalinkevich@gmail.com

Abstract ID #IMT-0795

Nanostructured surfaces are promisimg for the use in medical practice, industry, and defense, since such surfaces often have antibacterial properties, which is critical in the fight against biofouling, premature corrosion, and the preservation of cultural heritage. Chitosan, a natural polymer, has antibacterial and good film-forming properties, which allows it to be used to create film wound dressings in medicine, antibacterial biodegradable food films, as well as to create antibacterial coatings on other materials in order to increase biocompatibility or protect against environmental factors, including harmful bacteria. Strengthening the bactericidal effect can be achieved by structuring the surface. The combination of surface charge and certain structuring can enhance the antibacterial effect of a surface.

Chitosan films without and with magnetron sputtering were modified with a femtosecond laser, and their physicochemical and antibacterial properties were studied.

Chitosan (300 kDa, deacetylation degree 87%) films were prepared by pouring onto a substrate followed by evaporation of the solvent. Coatings were deposited on the chitosan film by magnetron sputtering using various carrier gases (nitrogen, oxygen) or vacuum. RF discharge frequency of 13.5 MHz, RF discharge power of 200 W, working gas (Ar) pressure of 1 Pa and a target-substrate distance of 7 cm. Coating thickness was 10–30 nm. A Ti : sapphire laser (Quantronix-Integra-C) system (pulse duration τ = 130 fs at a central wavelength of λ = 800 nm, repetition rate of 0.5 kHz, number of applied laser pulses N = 2, 10) was used for femtosecond for laser microprocessing of the samples.

Lasers can generate surface topographies of various geometries and sizes. Laser-created adhesions prevent bacterial aggregation by either killing them or preventing attachment by reducing the area of surface contact with bacteria.

Two Dimensional Metal Nanoplates Film for Electromagnetic Interference Shielding

Dong Su Lee *

" Institute of Advanced Composite Materials, Korea Institute of Science and Technology (KIST), Wanju-gun" (Republic of Korea)

* d.s.lee@kist.re.kr

Abstract ID #IMT-0835

The development of electromagnetic interference (EMI) shielding materials is essential for protecting electronic devices, ensuring signal integrity, and safeguarding human health and supports the advancement of emerging technologies such as 5G telecommunication, electric vehicles, and wearable electronics. There has been remarkable progress in the development of EMI shielding materials utilizing diverse nanomaterials [1-3]. However, in practical applications, metal-based thin films, foils, and meshes continue to be widely used for various advanced electronic device components, including components for flexible printed circuit boards.

In this study, single-crystalline copper nanoplates (CuNPs) were synthesized uisng a conventional hydrothermal method with copper chloride dihydrate ($CuCl_2 \cdot 2H_2O$), hexadecylamine, glucose, and iodine [4,5]. The CuNPs mixed in chloroform were spray-printed on a polyimide substrate. Through random deposition and layer-by-layer assembly, a hierarchically structured porous copper film was formed.

The CuNPs films demonstrated excellent EMI shielding performance compared to dense copper or other materials of the same thickness. They exhibited EMI shielding effectiveness (SE) values of 100 and 60.7 dB at thicknesses of 15 and 1.6 μm, respectively. The strong absorption of electromagnetic waves is attributed to the internal layer-by-layer stacked structures of the CuNPs and the multiple reflection effect within them, as demonstrated by FDTD simulations. The behavior is reminiscent of MXene materals [3]. These findings indicate that CuNPs fims hold great promise as potential EMI shielding materials for use in emerging technologies.

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Synthesis and Characterization of CuO Nanoparticles to Remove Heavy Metals

Ruth Condori, Maribel Guzman*, Betty C. Galaretta

Pontifical Catholic University of Peru (Peru)

* mguzman@pucp.edu.pe

Abstract ID #IMT-0841

Contamination of water by heavy metals has become a serious environmental problem around the world [1]. Among the various methods for removing heavy metals from polluted water, nanomaterials seem to be an interesting alternative for use it [2]. For this reason, the possibility of using copper oxide nanoparticles to remove cadmium ions will be evaluated [3-5]. Cupric oxide nanoparticles were prepared by the chemical precipitation method. The samples obtained were characterized by scanning electron microscopy-energy dispersive X-ray spectroscopy (SEM-EDS), X-ray diffraction (XRD), Raman and transmission electron microscopy (TEM). The results confirmed the formation of CuO with tenorite monoclinic structure. The crystallite size determined with the Scherrer formula was 19.74 nm. The nanoparticles obtained present spherical morphology with sizes between 18 and 68 nm. Finally, the cadmium removal assay shows that up to 7.5 % of Cd could be removed.

ACKNOWLEDGMENTS

This research work has been supported by the Master's program in Engineering and Materials Science, the grant "Seed Fund" (FGR-AG2042) of the academic department of Engineering and the facilities of the Materials Characterization Center (CAM) of Pontifical Catholic University of Peru.

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Nickel Nanowires Decorated with Palladium Nanoparticles as Powerful Catalysts Facilitating Synthesis of Polyfluorene Derivatives by Suzuki Polycondensation

Tomasz Wasiak[1 *], Dominik Just[2], Andrzej Dzienia[2, 3], Dariusz Łukowiec[4], Stanisław Wacławek[5], Anna Mielańczyk[1], Dawid Janas[2]

[1] *Silesian University of Technology, Faculty of Chemistry (Poland)*
[2] *Department of Chemistry, Silesian University of Technology, B. Krzywoustego 4, Gliwice (Poland)*
[3] *Institute of Materials Engineering, University of Silesia in Katowice, Bankowa 12, 40-007 Katowice (Poland)*
[4] *Silesian University of Technology (Poland)*
[5] *Technical University of Liberec, Institute for Nanomaterials (Czech Republic)*
* tomasz.wasiak@polsl.pl

Abstract ID #IMT-0864

Conjugated polymers are promising tools to differentiate various types of semiconducting carbon nanotubes (s-CNTs) [1]. However, their synthesis is a challenging issue. Lacks of control over molecular masses, irregular and unrepeatable batches hinder possible applications and scale-up [2]. Furthermore, commercial homogeneous catalysts often require an inert atmosphere and their recycle is almost impossible. To overcome those problems, modern catalytic systems are being developed. Here we present nano-based catalyst consisting of magnetic nickel nanowires decorated with highly active palladium nanoparticles. We used two-step wet chemical reduction protocol with assistance of sonochemistry, to obtain heterogeneous catalyst capable of conducting step-growth Suzuki polymerization of fluorene-derivatives. Additionally, we were able to boost the performance of our catalytic system by applying microwave irradiation in controlled manner. We studied the influence of main parameters on yield and polymer chain length, which provides more information about processes occurring in presence of metallic species under microwave irradiation. Produced polymers were used to extract semiconducting nanowires by polymer-wrapping methodology. Those results imply that development of a proper catalyst is crucial for controlling the synthesis of conjugated polymers. Furthermore, elimination of inert atmosphere simplifies the process and scale-up. Lowering cost and improving homogeneity of each batch will benefit the separation of s-CNTs, which can be used in wide spectrum of electronic devices such as sensors [3] and thin film transistors [4].

ACKNOWLEDGMENTS

The authors would like to thank the National Science Centre, Poland (under the SONATA program, Grant agreement UMO-2020/39/D/ST5/00285) for supporting the research

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The Electrostatic Control of the Exciton Radiative Lifetime in Quasi Type-II CdSe/CdS Two-Headed Nanostar

Grigor Mantashian *, Paytsar Mantashyan

A.B. Nalbandyan Institute of Chemical Physics NAS RA, 5/2 Paruyr Sevak St, Yerevan 0014 (Armenia)

* grigor.mantashian@gmail.com

Abstract ID #IMT-0889

Quantum dots (QDs) have captivated the attention of scientific community due to their diverse applications in nanophotonics, quantum information, optical sensing, and biolabeling [1, 2], derived largely from the size quantization effect. This effect engenders a discrete energy spectrum and alters the confined particle's probability density, both of which can be modulated by manipulating QD size, morphology, and applied external fields. Yet, a significant gap exists between experimental results and theoretical understandings in the field of manufacturing multilayer QDs of varied geometries and compositions, emphasizing the need for robust numerical modeling. However, traditional numerical methods, rooted in quantum chemistry, present challenges with respect to computational resource requirements and the flexibility to modify initial parameters like the geometry shape of the structure or the amplitude of the electric fields. This work advocates for the use of the finite element method (FEM) as a compelling alternative due to its balanced performance in accuracy and computational efficienc [3]. In this context, we employ FEM to examine the radiative excitonic lifetime of an exciton confined in a CdSe/CdS Two-Headed Nanostar with a quasi type-II band alignment. We define the band structure through a piecewise Woods-Saxon potential, enabling the tuning of the core radius and establishing a quasi type-II band alignment, resulting in a substantial reduction in the overlap between the electron and hole wavefunctions. Additionally, the overlap can be further managed by applying an electric field in the z-direction, given its disparate impact on the electron and hole. As the overlap strongly influences the exciton's radiative lifetime and overall optical properties, we meticulously investigate the control of the exciton radiative lifetime by varying the electric field intensity over different core radii. In the following article, the control of the exciton radiative lifetime is investigated by changing the electric field intensity in the range of $F=5*10^5$-$3*10^6$ V/m different core radii 2.2 nm - 4 nm. The obtained radiative lifetimes in the absence of the electric field are 37 ns which is close to the experimentally obtained results for a CdSe/CdS dot in rods [4].

Our research leverages the finite element method (FEM) to enhance understanding of quantum dots (QDs) and their role in nanophotonics and nanoscale devices, potentially revolutionizing diagnostics, imaging, and treatment in nanobiomedical applications. However, the versatility and efficacy of our FEM-based approach require further evaluation across a wider array of nanomaterials and external field conditions. While promising in theory, the practical applicability of these insights in nanophotonics, nanosensors, and nanodevices demands additional experimental validation.

ACKNOWLEDGMENTS

This work was funded by the Armenian National Science & Education Fund 2023 Yervant Terzian ANSEF Award: 23AN:PS-nano-2870.

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