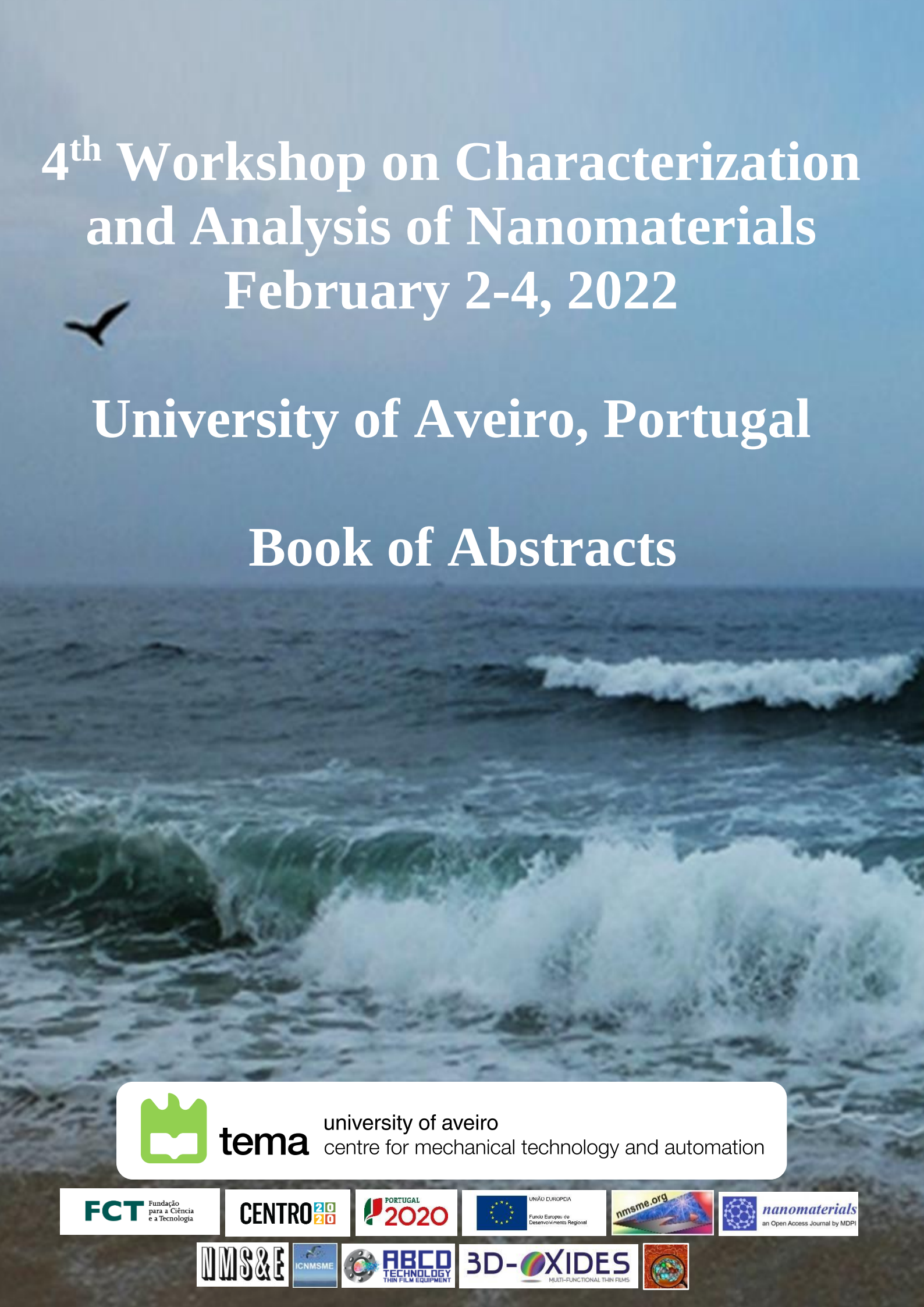
4th Workshop on Characterization and Analysis of Nanomaterials
February 2-4, 2022

University of Aveiro, Portugal

Book of Abstracts



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Gil Gonçalves
Raul Simões

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4th Workshop on Characterization and Analysis of Nanomaterials, February 2-4, 2022, University of Aveiro, Portugal (4th WCANM-2022)

Progress in science depends mainly on the level of experimental technology. Currently, interest in nanomaterials has led to many technological advances and has opened new horizons in understanding nature. Success in these ways was achieved by the development and standardization of methods for determining the characteristics of nanomaterials: X-ray diffraction, electron microscopy, atomic force microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, modelling of nanostructures, etc. A thorough knowledge of these methods is a necessary basis for work in modern science. The major aim of this workshop is to give a detailed description of principles and current state of the art of basic methods for the characterization of nanomaterials.

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Work program

February 2, 2022

4th Workshop on Characterization and Analysis of Nanomaterials, February 2-4, 2022, University of Aveiro, Portugal (*online*) **Auditorium 1**	
9:00-9:15	**WELCOME ADDRESS** **Prof. Dr. António Manuel de Bastos Pereira, Dr. Igor Bdikin**
9:15-10:15	CHAIR: Dr. Francisco Loureiro **The Computational Microscope: a Versatile Tool to Understand and Design NanoMaterials** **Prof. Dr. Manuel Melle-Franco** *CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Portugal*
10:15–10:35	**O10. Accurate prediction of COF structure from ab-initio methods** **Dr. Karol Strutyński** *CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal*
10:35–10:45	**Coffee break / Open discussions**
10:45–11:45	CHAIR: Dr. Francisco Loureiro **Raman Imaging: SERS studies and biodetection** **Prof. Dr. Helena Isabel Seguro Nogueira** *University of Aveiro, CICECO and Chemistry Department, Aveiro, Portugal*
11:45–12:05	**O8. Understanding Molecular Electrical Rectification** **Dr. Sara Gil Guerrero** *CICECO, University of Aveiro, 3810-193 Aveiro, Portugal*
12:05–12:25	**O7. 3D Polymerized C60** **Jorge Laranjeira** *Departamento de Física and CICECO, Universidade de Aveiro, Aveiro, Portugal*

12:25–12:55	**I1. Molecular modeling and physical properties of the peptide helical nanotubes based on the leucine, isoleucine amino acids** **Prof. Dr. Vladimir Bystrov** *Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia*
12:55–13:15	**O3. 2D MoS_2-Based Nanomaterials for Biosensing Applications** **Gurjeet Kaur** *Academy of Scientific and Innovative Research (ACSIR), Ghaziabad, India* *CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), India*
13:15–14:00	**Lunch break**
14:00–15:00	CHAIR: Dr. Gonzalo Guillermo Otero **Towards Quantitative Piezoresponse Force Microscopy measurements: Theory and Experiment** **Prof. Dr. Denis Alikin** *School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg, Russia*
15:00–15:20	**O6. Deposition of hexagonal $LuFeO_3$ thin films for photovoltaic applications** **Abderrazzak Ait Bassou** *CQVR, Physics Dep., ECT, Univ. Trás-os-Montes e Alto Douro, Vila Real, Portugal*
15:20–15:40	**O13. Development of a SERS-active nanopipette for scanning ion-conducting microscopy** **Aleksei Overchenko** *National Research University of Electronic Technology "MIET", Moscow, Russia*
15:40–16:00	**O11. Stability of PVP AgNPs in media of interest for polyelectrolyte multilayer build-up** **Ana-Marija Milisav** *Ruđer Bošković Institute, Zagreb, Croatia*
16:00–16:20	**Coffee break / Open discussions**

16:20–17:00	CHAIR: Dr. Gonzalo Guillermo Otero **Chemical beam vapor deposition technique with Sybilla equipment: review of main results in its 20-year anniversary** **Dr. Giacomo Benvenuti** *3D-Oxides, 130 rue Gustave Eiffel, F-01630 Saint-Genis-Pouilly, France* *ABCD Technology, Route de Champ-Colin 12, CH-1260 Nyon, Switzerland*
17:00–17:20	**O15. Chemical Synthesis of Gold Nanoparticles of Varying Shapes, Sizes, and Color for the Development of Lateral Flow Immunochromatographic Assay** **Dr. Bilal Javed** *School of Food Science and Environmental Health, College of Sciences and Health, Technological University Dublin, Dublin, Ireland* *Nanolab, FOCAS Research Institute, Technological University Dublin, Dublin, Ireland*
17:20–18:30	CHAIR: Dr. Igor Bdikin **P1-P14 (posters)**

February 3, 2022

4th Workshop on Characterization and Analysis of Nanomaterials, February 2-4, 2022, University of Aveiro, Portugal (*online*) **Auditorium 2**	
9:00-9:30	CHAIR: Dr. Natália Barroca **I2. Thin Layered nanostructured MoS_2 for photocatalytic applications** **Prof. Dr. Vikram Pandit** *Department of Chemistry, Haribhai V. Desai College, Pune-411002, India*
9:30-9:50	**O9. Nanocomposite of iron oxide and tin oxide for photocatalytic application** **Ragini Ahiwale** *Department of chemistry, Haribhai V. Desai college, pune-411002, India*
9:50–10:00	**Posters/ Coffee break / Open discussions**
10:00–11:00	CHAIR: Dr. Natália Barroca **Temperature induced phase transition in crystal and magnetic structure of $BiFe_{1-x}MnxO_3$ ceramics** **Prof. Dr. Dmitry Karpinsky** *National Research University of Electronic Technology "MIET", Zelenograd, Russia* *Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus*
11:00–11:20	**O17. Nanocrystalline YSZ Electrolyte by coprecipitation for Solid Oxide Fuel Cell** **Prerna Vinchhi** *Department of Solar Energy, School of Technology, Pandit Deendayal Energy University, Gandhinagar, India*
11:20–11:40	**O4. Flexible thermoelectric generator based on Bi-Te-Se and Bi-Sb-Te materials** **Irina Voloshchuk** *National Research University of Electronic Technology, Zelenograd, Moscow, Russia*
11:40–12:00	**O14. Formation of sensitive elements based on titanium dioxide nanowires by the direct ink writing method** **Andrey Tarasov** *National Research University of Electronic Technology "MIET", Moscow, Russia*

12:00–12:40	**SAS 3D OXIDES** **Dr. Giacomo BENVENUTI** *3D-Oxides, 130 rue Gustave Eiffel, F-01630 Saint-Genis-Pouilly, France*
12:40–13:00	**O2. Synthesis and Characterization of Magneto-Fluorescent Nanoparticles and its application in food safety** **Saloni Sharma** *Academy of Scientific and Innovative Research, Ghaziabad, 201002, India* *CSIR-Central Scientific Instruments Organisation, Sector-30, Chandigarh, 160030, India*
13:00–14:00	**Lunch break**
14:00–14:30	CHAIR: Dr. Gil Gonçalves **Modeling and calculations of the hydroxyapatite structures with various defects** **Dr. Ekaterina Paramonova** *Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, Pushchino, Moscow 142290, Russia*
14:30–15:30	**Magnetic characterization methods of nanomaterials** **Prof. Dr. Paulo C. DE MORAIS** *Catholic University of Brasília, Brazil &University of Brasília, Brazil*
15:30–16:10	**ABCD TECHNOLOGY** **Dr. Giacomo BENVENUTI** *ABCD Technology, Route de Champ-Colin 12, CH-1260 Nyon, Switzerland*
16:10–16:30	**Coffee break / Open discussions**
16:30–16:50	CHAIR: Dr. Gil Gonçalves **O1. Computer modeling and numerical studies of peptide nanotubes based on diphenylalanine** **Dr. Sergei Filippov** *Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, Pushchino, Moscow 142290, Russia*

16:50–17:10	**O12. Self-cleaning SERS substrate based on ZnO nanorods and supported by Ag nanoparticles** **Denis Novikov** *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia*
17:10–17:30	**O5. Synthesis and characterization of Magnetite-hydroxyapatite-clay Removal of Contaminants from wastewater** **Ayoub Grouli** *Laboratory of Analytical And Molecular Chemistry, Department of Chemistry, Faculty of Sciences Ben M'sick, University Hassan II of Casablanca, Morocco*
17:30–17:50	**O16. Rapid Detection of Salmonella by using Antibody Functionalized Immuno-magnetic Iron Oxide Nanoparticles** **Dr. Bilal Javed** *School of Food Science and Environmental Health, College of Sciences and Health, Technological University Dublin, Dublin, Ireland* *Nanolab, FOCAS Research Institute, Technological University Dublin, Dublin, Ireland*
17:50–18:30	**Final discussions and comments**

* Lectures on basic characterization methods are highlighted in green.
** Presentations of companies produce equipment for characterization materials are highlighted in yellow.

Poster session, 17:20–18:30, February 2, 2022

P1	**Specificities of adsorption properties of nanocomposites of multiwalled carbon nanotubes and polyamide, polyethylene, polyvinyl chloride, expanded polystyrene** A. P. Onanko, D. V. Charnyi, Y. A. Onanko, O. P. Dmytrenko, M.P. Kulish, T. M. Pinchuk-Rugal, P. P. Ilyin *Kyiv national university, Kyiv, Ukraine*
P2	**Investigation of thermoelectric properties and thermal stability of low-temperature thermoelectric material based on Bi-Te-Se system** Dmitry Pepelyaev, Maxim Shtern, Maxim Rogachev, Yury Shtern, Alexey Sherchenkov, Alexey Babich *National Research University of Electronic Technology, Bld. 1, Shokin Square, Zelenograd, Moscow, Russia*
P3	**Investigation of the crystallization kinetics for thin films of phase change memory material Ge2Sb2Te5** A. Bozhedomova, A. Babich, A. Sherchenkov, D. Glebova, A. Yakubov, M. Fedyanina *National Research University of Electronic Technology, Bld. 1, Shokin Square, Zelenograd, Moscow, Russia*
P4	**Methods for obtaining nanostructured thermoelectric materials on the basis of Bi2Te3 and Sb2Te3 for temperature range of 200-500 K** M.Yu. Shtern, M.S. Rogachev, Yu.I. Shtern, A.A. Sherchenkov, E.P. Korchagin, B.R. Mustafoev *National Research University of Electronic Technology, Shokin Square 1, Zelenograd, Moscow, 124498, Russia*
P5	**Thermal conductivity of nanostructured thermoelectric materials on the basis of PbTe and GeTe** M.Yu. Shtern, M.S. Rogachev, Yu.I. Shtern, A.A. Sherchenkov, E.P. Korchagin, B.R. Mustafoev *National Research University of Electronic Technology, Shokin Square 1, Zelenograd, Moscow, 124498, Russia*
P6	**Nanocomposite of Iron Oxide and Titanium Oxide for Photocatalytic applications** Ganesh Jadhav, Vikram Pandit *Department of Chemistry, Haribhai V. Desai College, Pune-411002, India*
P7	**Influence of thin-film heat sinks and barriers on the combustion of Al-CuOx multilayer thermites** E.A. Lebedev, M.E. Shiryaev, A.V. Sysa, R.M. Ryazanov, D.G. Gromov *National Research University of Electronic Technology – MIET, Moscow, Zelenograd, Russia; Scientific-Manufacturing Complex "Technological Centre", Moscow, Zelenograd, Russia*

P8	**Structure and functional properties relationship in Sc-doped LuFeO3** Anton Turygin, Denis Alikin, Aliaksandr Zhaludkevich, Andrei Ushako, Andrius Pakalniškis, Aivaras Kareiva, Dmitry Karpinsky *School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg, Russia; SSPA «Scientific-Practical Materials Research Centre of NAS of Belarus», Minsk, Belarus*
P9	**Photocatalytic degradation of caffeine using graphitic carbon nitride as the catalyst** Martina Kocijan, Lidija Ćurković, Tina Radošević, Damjan Vengust, Matejka Podlogar *Department of Materials, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia; Department for Nanostructured Materials, Jožef Stefan Institute, Jamova Cesta 39, SI-1000 Ljubljana, Slovenia; Advanced Materials Department, Jožef Stefan Institute, Jamova Cesta 39, SI-1000 Ljubljana, Slovenia; Department of Chemical Engineering and Technical Safety, Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna Pot 113, SI-1000 Ljubljana, Slovenia*
P10	**Self-cleaning SERS-active substrates using a Si-compatible process flow** H. Bandarenka, S. Dubkov, D. Gromov, A. Savitsky, D. Novikov, A. Tarasov, S. Zavatski, K. Girel, A. Burko, A. Liashchynskaya, A. Borisiyuk *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Belarusian State University of Informatics and Radioelectronics, Minsk, Belarus*
P11	**Fabrication silver/hafnium oxide nanostructures on the macroporous silicon as SERS-active substrates** K. Girel, K. Litvinova, A. Burko, S. Dubkov, A. Savitsky, D. Novikov, A. Tarasov, H. Bandarenka *Applied Plasmonics Laboratory, Belarusian State University of Informatics and Radioelectronics, Minsk, Belarus; Institute of Advanced Materials and Technologies, National University of Electronic Technology, Moscow, Russia; National University of Science and Technology MISIS, Russia*
P12	**Formation of niobium oxide thin films by reactive magnetron sputtering** E. Grinakovskiy, D. Gromov *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia*
P13	**Synthesis of barium titanate nanowires for a piezoelectric actuator** Vu Van Zung, S. Dubkov, D. Gromov, A. Tarasov, A. Savitskiy, R. Ryzanov *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Scientific-Manufacturing Complex «Technological Centre», 124498 Moscow, Russia*
P14	**Electromechanical properties of compounds based on BiMnO3** S.I. Latushka, D.V. Zhaludkevich, V.V. Sikolenko, T.V. Latushka, D.A. Kiselev, P.A. Sklyar, D.V. Karpinsky *Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus; Joint Institute for Nuclear Research, Dubna, Russia; Belarusian State Medical University, Minsk, Belarus* *4National University of Science & Technology "MISiS", Moscow, Russia*

Centre for Mechanical Technology Automation (TEMA), Department of Mechanical Engineering, University of Aveiro

In a world of constant change, the capacity of adjustment is essential. The Centre for Mechanical Technology and Automation (TEMA) is highly aware of this factor and fully comprehends the relevance of the R&D conducted in the research unit and its impact on society (academic, industrial/business and civil) and is experiencing a crucial transition period of structural adaptation to ensure the continued pursuit of scientific excellence with a contextualized translation in(to) innovation, competitiveness and citizenship of the community. This transition aims to ensure the essence of TEMA and to capitalize the background of expertise of its members that is enriched by the diversity of scientific fields, distributed in six main areas of knowledge: applied mechanics; applied energy; biomechanics; modelling & simulation; nanoengineering and transportation technologies.

Based on its Human Capital and Capacities, the Centre for Mechanical Technology and Automation (TEMA) embraces a mission aiming to contribute to a sustainable industry, with specially focus on the surrounding SMEs, and to the wellbeing of society. This is pursued by the development of excellence, cutting-edge and high impact research and innovation in engineering and technology, a mission made possible by the Researchers that compose TEMA, together with a responsible and effective fulfillment of the strategic mobilizing projects.

TEMA is focused on current societal challenges and upcoming global requirements, translated into three main mobilizing projects (MP): Mobilizing Project 1 – Sustainable Manufacturing Solutions; Mobilizing Project 2 - Technologies for the Wellbeing; and Mobilizing Project 3 - Research Infrastructure, involving TEMA's members as one coherent group. MP1 is focused on the development and innovation on manufacturing engineering and technologies, with subsequent industrial applications. It is intended to increase productivity, improve products' quality, and reduce waste in production processes. The strategy of the MP2 aims to increase the quality of life of society by means of engineering systems, focusing on people and their needs. MP3 aims at a rational and efficient management of TEMA's material and human resources (including its 14 laboratories), its vast array of scientific equipment in a large diversity of areas available to society, making the research infrastructure an "open facility" for a number of (academic, research and industry) end-users.

Prof. Dr. António Manuel de Bastos Pereira
Director of TEMA - Centre for Mechanical Technology and Automation

Plenary lectures

Raman Imaging: SERS studies and biodetection

Helena Nogueira*, Sara Fateixa, Tito Trindade

University of Aveiro, CICECO and Chemistry Department, Aveiro, Portugal
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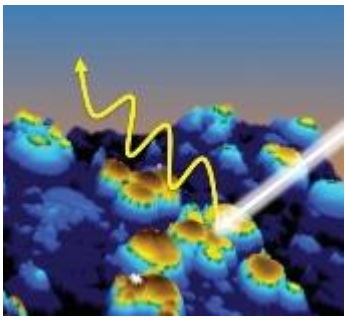
Surface-enhanced Raman scattering (SERS) allows selective detection that can be used for biological sensing, combining the capability of molecular fingerprinting with very high sensitivity. The assembly of metal nanoparticles, silver and gold in particular, into suitable substrates for SERS sensing has been intensively investigated [1]. We have been focused on the preparation of silver and gold nanocomposites, by supporting the metal nanoparticles in a variety of matrices such as graphene, polymers and textiles [2,3]. The current developments of techniques such as Raman imaging, through high resolution confocal Raman mapping with short measurement times, have brought a new look on nanocomposites and SERS applications. A Raman image can show either the chemical heterogeneity of the nanocomposite or a specific response such as SERS activity or a labeling process (Figure 1).



In this communication, our latest results in the development of SERS active substrates will be presented together with its evaluation using Raman imaging. Illustrative examples of SERS applications will be provided along with perspectives of development in chemical detection applied to real contexts. There has been an interest in developing new SERS substrates that make this type of analysis handy, versatile and faster. Polymer based silver or gold nanocomposites can be used as SERS substrates in versatile solid films or in aqueous emulsions. The possibility to obtain SERS using Ag/PtBA (poly-tert-butylacrylate) nanocomposites as substrates was investigated in detail. SERS activity for the detection of DNA nucleobases and DNA itself will be presented.

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[3] N. Martins, S. Fateixa, T.Fernandes, H. Nogueira, and T. Trindade, *ACS Applied Nano Materials*, **4**, 4484 (2021).

Magnetic characterization methods of nanomaterials

Paulo C. DE MORAIS
Catholic University of Brasília, Brazil
&
University of Brasília, Brazil

The talk is addressed to present and discuss a collection of magnetic-based experimental techniques widely used for characterization of magnetic nanomaterials. Among the available experimental techniques, the hysteresis cycle, AC- and DC-susceptibility, FC- and ZFC-measurements, ferromagnetic resonance and Mossbauer spectroscopy are selected for presentation and discussion. In addition to the experimental results, analyses of the experimental data related to each of the selected techniques will be presented. The talk will explore different approximations, based on model pictures interconnected to each other, which provide the protocols for the experimental data analyses.

Towards Quantitative Piezoresponse Force Microscopy measurements: Theory and Experiment

Denis Alikin[1,*], Mikhail Kosobokov[1], Lyubov Gimadeeva[1], Artur Udalov[1], Boris Slautin[1], Alexander Tselev[2], Andrei Kholkin[1,2]

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Piezoresponse force microscopy (PFM) is a local technique allowing measurement of the surface piezoresponse with a uniquely high spatial resolution in the micro and nano-objects where macroscopic measurement techniques fail and PFM becomes the only way to quantify the material's piezoelectric coefficients. In PFM mode, the electric field is applied to the scanning probe microscopy probe with a radius of tens nanometers, which creates a highly inhomogeneous electric field. This makes the measurements much more complicated compared to the case of the uniform electric field and related electromechanical deformation inside the piezoelectric capacitor [1]. PFM measurements possess many uncertainties, such as a significant impact from the electrostatic force, the drop of the applied voltage across the tip-surface interface, mechanical clamping of the oscillating surface, etc.

In this report, we discuss possibilities to quantify PFM, i.e., get reliable and calibrated piezoresponse values and extract the information about real components of the piezoelectric tensor. This complicated problem includes technical difficulties, experimental and theoretical issues. Here, we explain how to set up PFM to collect reliable data in the experiments and discuss the theoretical framework of piezoelectric coefficients evaluation from PFM data. The most important data treatment in PFM spectroscopy and microscopy is illustrated. We also introduce fully quantitative "global-excitation" mode PFM allowing accurate recovery of the piezoelectric coefficient in the micro-scale objects.

The work is supported by the Russian Science Foundation (grant 19-72-10076).

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[1] A. Udalov, D. Alikin, and A. Kholkin, *Sensors*, **21**, 3707 (2021)

The Computational Microscope: a Versatile Tool to Understand and Design NanoMaterials

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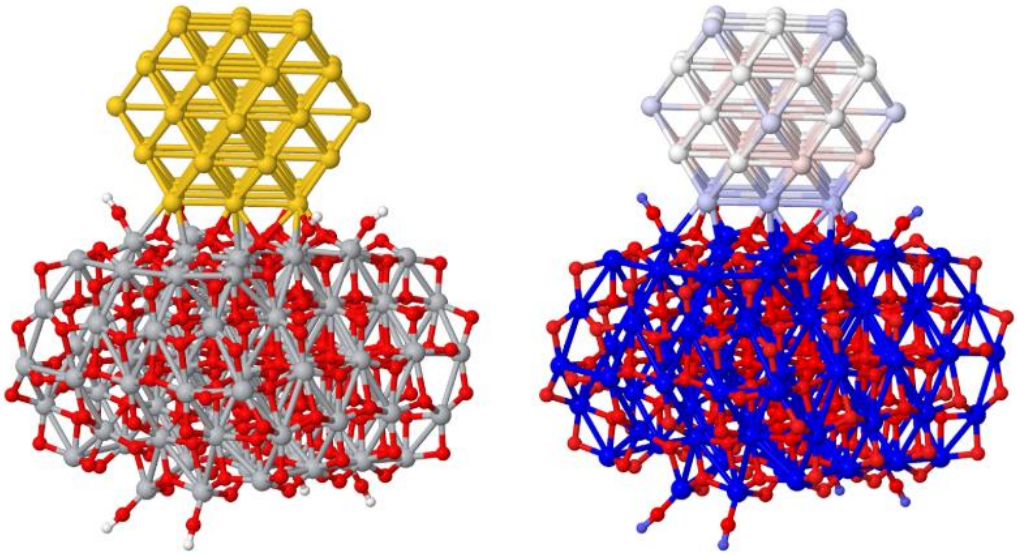
Computer modelling has become a key feature to understand and predict existing and new materials and molecules. From our extensive experience applying and developing computational models, we will illustrate through examples how computer models have evolved and yield key information on diverse problems in nanoscience such as magnetic and bottom-up nanographenes, covalent organic frameworks [1], and composites based on inorganic nanoparticles [2] and peptides [3].



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[2] Enhanced Activity of Au/TiO2 Nanoparticles against Ciprofloxacin. *Catalysts* **10**, 234 (2020)
[3] Oxidized Nanocarbons-Tripeptide Supramolecular Hydrogels: Shape Matters! *ACS Nano* **12**, 5530–5538 (2018).

Modeling and calculations of the hydroxyapatite structures with various defects

V. S. Bystrov[1,*], **E. V. Paramonova[1]**, L. A. Avakyan[2], J. Coutinho[3]

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This review provides an analysis of the developed methods and approaches for modeling and calculating hydroxyapatite (HAP) with defects. This is important for many HAP applications. Thus, calculation methods were developed using the density functional theory (DFT) based on the semilocal exchange-correlation functional (PBE) and hybrid functionals (B3LYP, HSE), including a 2-stage method for calculating the energetics of HAP structures [1]. Using these DFT methods, extensive calculations were performed on models of both initial stoichiometric HAP crystals and optimized HAP structures, and HAP structures with various defects (in particular, oxygen vacancies of different groups, hydroxyl group vacancies, with Sr/Ca substitutions, substitutions and interceptions with iron ions Fe2+, Fe3+, etc.). Based on these developed DFT methods and approaches, using them both for models of one primitive HAP cell ($P6_3$ and $P6_3/m$) and models of supercells from (8 = 2x2x2 cells), structural and energy band characteristics of HAP (cell parameters, band gap; energy levels created by defects), the structural, mechanical, electronic and optical properties of HAP, both of the ideal stoichiometric structure of HAP and HAP structures with various defects, have been calculated. An analysis of the results of calculations using various software tools (AIMPRO, VASP, Quantum ESPRESSO) showed their good agreement.

In addition, a classification of defects in the formation of oxygen vacancies from different PO4 and OH groups was developed and introduced, taking into account their positions and symmetry. The existence in HAP, in addition to ordinary point defects characteristic of neutral oxygen vacancies, extended (bridge) defects of a new type for charge states with a charge q=+2, was established.

A new method has been developed for calculating the energy characteristics of formed defects in hydroxyapatite, using the thermodynamic approach to describe them as quasiparticles in a solid. Calculations using this technique made it possible to refine and generalize the results obtained in the conventional Kohn-Sham density functional theory (DFT) in calculating the energies of the defect levels and optical transitions of electrons. The band gap Eg of the initially pure stoichiometric hydroxyapatite of the $P6_3$ hexagonal phase refined by this technique, which is ~7.3 eV in the Kohn-Sham DFT, becomes equal to ~6.85 eV, i.e., ~0.45 eV less. This is a new and fundamentally important result.

The application of this approach to calculating the optical properties of defects such as oxygen vacancies (of various types) and hydroxyl groups also made it possible to refine all the calculated values of optical transitions (including the effective band gap Eg* under photoexcitation, for example, in cases of different types of oxygen vacancies) and determine their values at the level Eg* ~ 3.6 - 4.3 eV, which turns out to be closer to the experimentally observed values in various experimental HAP samples. Taking into account the Franck-Condone effect has also been developed.

New results of calculations by the methods indicated above were also obtained for models of HAP structures containing defects of strontium substitution Sr/Ca in different

positions of calcium atoms Ca (I) and Ca (II). The main results are as follows: 1) The calculated data on structural changes (lattice constants and cell volume) upon substitution of Sr/Ca in HAP in comparison with the data showed a similar increase in all parameters of the HAP cell after replacing Sr/Ca; 2) Changes in optical properties (band gap Eg, etc.) after Sr/Ca substitution were studied, and an increase in the calculated band gap Eg after Sr/Ca substitution was noted. In this case, a corresponding increase in the electron work function was also found. This changes the HAP surface potential and stimulates the proliferation of osteoblast cells on HAP coated implants, ensuring the growth of bone tissue.

Calculations of defects in hydroxyapatite during the insertion/replacement of Ca and P atoms in the HAP lattice by Fe ions (taking into account their charges) have been performed. The defects were considered by model of an orthorhombic supercell consisting of 8 HAP unit cells $P6_3/m$ (352 atoms). The calculations were carried out by DFT methods using the Quantum ESPRESSO program according to 2-stage technique (PBE/HSE). It was shown that the most probable configurations of defects are: substitutions of Fe3+ and Fe2+ at Ca (I) and Ca (II) positions under conditions of low Ca content. Fe insertions at the edge of the hydroxyl channel of the hydroxyapatite structure are preferred in Ca-rich HAP. For the Fe-HAP structure, 26 models of defect configurations were considered. It is shown that the relaxation of the investigated structures leads to a number of new configurations of Fe-HAP structures, which were classified and studied in detail.

A representation was developed for the dependence of the energies of defect formation on the Fermi energy level with different charge states (in different cases of investigated defects in HAP) and at different charge states of the defects. This technique of "phase diagrams" makes it possible to analyze the regions of stable existence of various defects in hydroxyapatite, and it was applied to the analysis of OH group vacancies, oxygen vacancies of different types and charges, as well various types of Fe defects in HAP, were analyzed [2]. Iron-doped Fe-HAP is of interest due to its magnetic properties and biocompatibility. It is a promising material for magnetic resonance imaging, thermal centers for magnetic hyperthermia, sunscreen creams, antimicrobial coatings, and drug delivery systems. This work was supported by the RFBR grant 19-01-00519_a.

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Temperature induced phase transition in crystal and magnetic structure of $BiFe_{1-x}Mn_xO_3$ ceramics

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Crystal and magnetic structure of the compounds (1-x)BiFeO3-(x)BiMnO3 has been studied using synchrotron and neutron diffraction, magnetometry and differential scanning calorimetry. It has been found that increase in Mn content leads to the structural transition from the polar rhombohedral to the anti-polar orthorhombic and then to the monoclinic phase via two phase concentration ranges of the adjacent phases in the concentration range 0.25 < x < 0.30 and 0.60 < x < 0.65 respectively at room temperature (Figure 1).

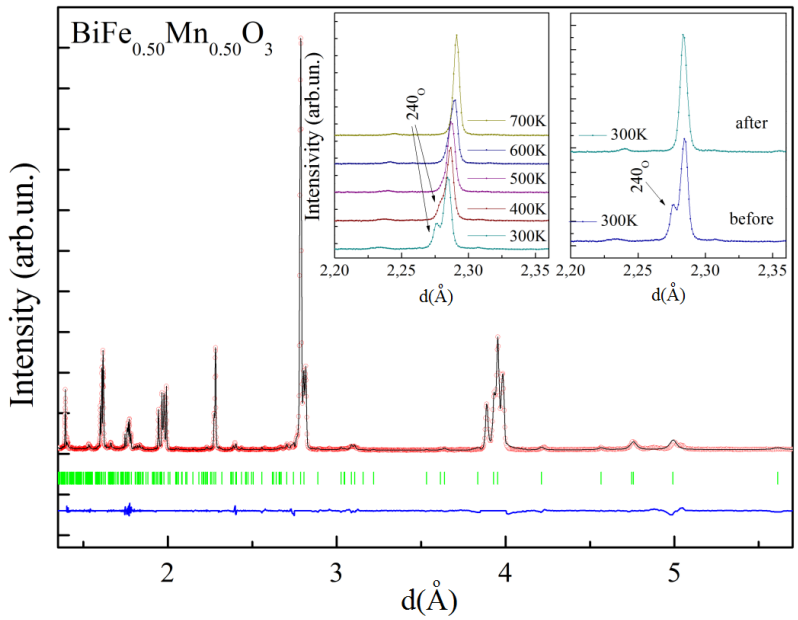

Figure 1. SPD pattern recorded for $BiMn_{0.5}Fe_{0.5}O3$ at room temperature, inset shows temperature evolution of the reflections specific for different structural phases

It is determined that concentration driven structural transition from the rhombohedral to the orthorhombic phase is accompanied with a destruction of the modulated anti-ferromagnetic structure towards the non-collinear antiferromagnetic structure ascribed as to weak ferromagnetism and then to orbitally ordered ferromagnetic structure. Annealing of the compounds at high temperatures (above 600 K) leads to the irreversible phase transitions favoring a stabilization of the structural phase stable at high temperatures. The magnetic states of the compounds subjected to high temperature annealing show notable changes caused by an increase in the amount of appropriate structural phase.

Acknowledgement

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Invited speakers

I1. Molecular modeling and physical properties of the peptide helical nanotubes based on the leucine, isoleucine amino acids

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This work presents models of the helix-like structure of dipeptide nanotubes based on amino acids such as leucine and isoleucine. Cases of different chirality of the initial amino acids (with left - “L” and right - “D”) and their influence on the formation of final peptide nanotubes strictures were considered. The paper analyzes the structural features of all types of PNT in comparison with experimental data. The results of calculations of the physical properties (dipole moments, polarization, piezoelectric coefficients, etc.) are also given. The main tool for molecular modeling of all studied nanostructures was the HyperChem 8.01 package. Various computational methods have been used such as molecular mechanics (MM) methods (including MM +, Amber, BIO CHARM), quantum mechanical (QM) self-consistent field (SCF) calculations, Hartree-Fock (HF) calculations, and various semi-empirical methods (PM3, AM1, RM1, ZINDO-1), using restricted Hartree Fock (RHF) and unrestricted Hartree Fock (UHF). For comparison and analysis of PNT structures, their structures constructed and calculated using density functional theory (DFT) by the VASP program (as well as Quantum ESPRESSO) based on experimental structural X-ray data from the CCDC database were then converted from the *.vasp, *.cif and *.pdb formats into *.hin HyperChem formats. Here, in the HyperChem working space, their main molecular structures, forming peptide helical nanotubes, were isolated, selected and investigated, and all their basic physical properties were calculated. It was found that for the experimental helix-like structures the values of the dipole moments and polarization turned out to be significantly higher (almost 2 times) than for model structures based on ring-like layers of nanotubes. These helical structures are energetically more favorable, therefore they can self-assemble from solutions with certain conditions in an aqueous medium. However, the structures of isoleucine can also form other non-tubular forms; these issues still require additional research. A comparison and analysis of the difference in the formed helical structures of nanotubes depending on the different types of chirality of the initial amino acids leucine and isoleucine were also performed. It was found that the formation of helix-like nanotubes has a chirality screw opposite to the original amino acids, that confirms the general law of the alternation of chirality types with the complication of structures in the self-organization of biomacromodecules. This work was supported by the RFBR grants 19-01-00519_a and 20-51-53014_GFEN_a.

I2. Thin Layered nanostructured MoS_2 for photocatalytic applications

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In the present study, Lawesson's reagent (LR) is used as a sulfur source for the formation of layered MoS_2 semiconductor nanostructures. MoS_2 layers are prepared using 15 hr. hydrothermal reaction method at 120°C. X-ray diffraction (XRD), UV-visible (UV), BET analysis and FESEM and TEM micrographs of 15 hr. reaction time. After synthesis and characterization, MoS_2 nanostructures were checked for its photocatalytic behavior. For photocatalytic study two complex organic dyes (Methylene blue and Crystal violet) degradation and water splitting experiments were carried out. MoS_2 degrades almost 71% and 57% of MoS_2-MB and MoS_2-CV, respectively within 90 min. of irradiation time in natural sunlight. Also, photocatalytic dye degradation found almost 82% and 73% of MoS_2-MB and MoS_2-CV, respectively within 90 min. of irradiation time in lab under artificial lamp. As compared to natural sunlight study the rate of dye degradation found more in UV lamp experiments for both the dyes.

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Oral presentations

O1. Computer modeling and numerical studies of peptide nanotubes based on diphenylalanine

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The paper presents the results of computer studies of the structural and physical properties of such self-organizing structures as peptide nanotubes based on diphenylanine dipeptide with different initial isomers of the left and right chiralities of these dipeptides. The structures under study are considered both with empty anhydrous and with internal cavities filled with water molecules.

Molecular models of both ring and spiral structures are investigated, which are consistent with the known experimental data.

To study the effect of nano-sized clusters of water molecules embedded in the inner hydrophilic cavity on the properties of nanotubes (including changes in their dipole moments and polarization), as well as changes in the structure and properties of water clusters themselves (their dipole moment and polarization) for both types of chirality, the surfaces of the cavities of nanotubes are analyzed. and outer surfaces of water cluster structures.

This was done using a specially developed visual differential analysis of the structural features of (bio)macromolecular structures [1].

The obtained results of calculations of a number of physical properties (polarization values, etc.) are given for various cases and analyzed in comparison with the known data. These data and the obtained structural features are necessary for the analysis of the interactions of water molecules with hydrophilic parts of nanotube molecules based on diphenylalanine, such as COO^- and $NH3^+$, since they determine many properties of the structures under study.

A number of the obtained data are planned to be used for further analysis of the possible adhesion and trapping of certain medical molecular agents (components) with active layers of nanotubes based on diphenylalanine, which can be useful for creating targeted delivery capsules of pharmaceuticals and drugs on their basis.

This work were supported by the RFBR grants 19-01-00519_a and 20-51-53014_GFEN_a.

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https://library.keldysh.ru/preprint.asp?id=2021-78

O2. Synthesis and Characterization of Magneto-Fluorescent Nanoparticles and its application in food safety

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Food safety has emerged as an important global issue as it impacts the wellbeing of individuals as well as nations. Food borne illness arisen from a bacterial pathogen like *Salmonella sp*. is a significant health concern. 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. Iron oxide nanoparticles have been extensively used due to their biocompatibility and minimal side effects. This work presents a unique combination of nano-sized magnetite nanoparticles (Fe_3O_4), surface functionalized with a silica shell and conjugated with Fluorescein isothiocyanate (FITC). The microwave assisted Fe_3O_4 nanoparticles were responsible for magnetic separation of the target analyte. The silica shell provided water stability and FITC was used as a fluorescence marker for the optical detection of *Salmonella sp*. To the synthesized nanoparticles, the *anti- Salmonella* antibody was immobilized through EDC-NHS carbodiimide crosslinking mechanism. The Fe_3O_4-Si-FITC functionalized nanoparticles were characterized by various analytical techniques such as XRD, FESEM, FTIR, Raman and UV spectroscopy. The optical response against *Salmonella sp.* was recorded through Photoluminescence Spectroscopy and the obtained results showed that the nanoparticle based platform was effective in the biosensing of food borne pathogen *Salmonella sp.*

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O3. 2D MoS_2-Based Nanomaterials for Biosensing Applications

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Molybdenum disulfide (MoS_2), a typical 2D layered inorganic material i.e., transition metal dichalcogenide, due to its unique structural, physicochemical, optical, and biological properties has received immense interest in the past few years. The distinctive structure and unique band gap make it a promising material to substitute graphene and other semiconductor devices. While MoS_2 has a broad range of energy applications in batteries, solar cells, microwave, and many other applications, its 2D and 0D forms have led to diverse applications in electronics especially sensors like optical sensors, biosensors, electrochemical biosensors that play an important role in the detection of various diseases. Herein, a systematic overview of the progress that is made in the field of MoS_2 research with an emphasis on its different biosensing applications is presented. This article provides a general discussion on the basic structure and properties of MoS_2 and discuss the latest research advancement with emphasis on its different morphologies that are synthesized so far, such as, nanosheets and quantum dots. The focus is on its biosensing applications and future challenges.

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O4. Flexible thermoelectric generator based on Bi-Te-Se and Bi-Sb-Te materials

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Recently, a new direction in thermoelectricity has appeared, which is associated with the active development of wearable electronics. Screen printing is one of the most promising technologies for the manufacture of flexible thermoelectric generators (TEG). However, this technology must be developed to obtain thermoelements with high thermoelectric and electrophysical properties. In particular, the optimal composition of the binder has not been determined. It is known that solid solutions based on Bi_2Te_3-Sb_2Te_3 (p-type) and Bi_2Te_3-Bi_2Se_3 (n-type) have a high thermoelectric efficiency as low-temperature thermoelectric materials (TEM).

Therefore, the aim of the work was to study the properties of thick films on the basis of Bi_2Te_3-Sb_2Te_3 and Bi_2Te_3-Bi_2Se_3 produced with using of an aqueous solution of alkaline sodium silicate (SS) and zinc phosphate cement (ZPC) as binders. In addition, the development, fabrication and investigation of a prototype of flexible thermoelectric generator fabricated with using the research results were carried out.

It has been established that the legs of thermoelements with film contacts, fabricated with using of SS have the best parameters. Their electrical conductivity was 20.00 and 14.00 $Ohm^{-1}\cdot cm^{-1}$ for p- and n-types, respectively, and the Seebeck coefficient was 250 μV/K for both types of conductivity. Therefore, this type of suspension was used to form thermoelement legs for the flexible TEG. A silicone-based flexible TEG was developed, fabricated and investigated. The developed TEG includes 6 pairs of n- and p-type legs. At room temperature (298 K), the output voltages of the flexible thick film TEG at ΔT = 2.5 and 10.0 K are 0.8 and 14.8 mV, respectively, which is not worse than the parameters of thick film TEGs presented in publications. Thus, the developed technology is promising and can be used to form legs of thermoelements for flexible TEGs.

This work was supported by Russian Science Foundation (project number 18-79-10231).

O5. Synthesis and characterization of Magnetite-hydroxyapatite-clay Removal of Contaminants from wastewater

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The synthesis of hydroxyapatite (HAP) and its composite by various techniques, are abridged by highlighting the green technique that involves the use of environmentally friendly solvents such as water and the substitution of precursors by waste Resources. Magnetic HA plays a major role in HA composites because of the ease of recovery and re-use. The composition and surface morphology of the resulting HA composite were studied in detail. The adsorptive removal of Cu(II) and methylene blue (MB) using HA-Bentonite was studied in different systems .

The results indicate that HA-Bentonite exhibits efficient removal of Cu(II) and MB with favorable adsorption at high pH. The mechanisms involved in the adsorption of Cu(II) and MB are electrostatic interaction and surface complexation.
The optimal conditions were found to be 3 g/L (adsorbent dosage), 10h (contact time contact time), 25 mg/L (initial Cu(II) concentration), and 85 mg/L (initial MB concentration).The adsorption kinetics and equilibrium fit well with the Elovich and Langmuir models, respectively. Desorption studies confirmed that the HA-Bentonite adsorbent can be regenerated and reused efficiently.

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O6. Deposition of hexagonal $LuFeO_3$ thin films for photovoltaic applications

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The Lu-Fe-O system has several phases with technological interest, such as the $Lu_3Fe_5O_{12}$ garnet, the orthorrombic *o*-$LuFeO_3$ perovskite and the hexagonal *h*-$LuFeO_3$ [1]. The latter is a ferroelectric metastable phase with a theoretical direct bandgap around 1.8 eV which makes it promising for photovoltaic ferroelectric applications. So far only a few reports of band gap measurements in *h*-$LuFeO_3$ thin films are available [2].

In this work, thin films of the Lu-Fe-O system were deposited on silica glass and on (Si(100)/SiO_2/TiO_x/Pt) substrates by Aerosol-assisted Metalorganic Chemical Vapour Deposition (MOCVD). $Lu(tmhd)_3$ and $Fe(tmhd)_3$ were used as metalorganic precursors.

As the *h*-$LuFeO_3$ is a metastable phase, different deposition temperatures (600-800°C) were tested. The development of the *h*-$LuFeO_3$ phase was best achieved performing a deposition as an amorphous film at 700°C and latter inducing the crystallization of the *h*-$LuFeO_3$ phase by an *ex-situ* thermal treatment at 850°C. The deposited films were characterized by X-ray diffraction, scanning electron microscopy (SEM) with EDS, atomic force microscopy (AFM), Raman spectroscopy and by optical techniques (UV-Vis). Values of 1.80 eV for direct and indirect band gap were obtained which agree with the ones pointed out by Holinsworth [2].

We can conclude that thin films of the h-$LuFeO_3$ phase have a promising potential application in ferroelectric photovoltaic devices.

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O7. 3D Polymerized C_{60}

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Three-dimensional (3D) C60 polymerized structures with each molecule adopting one of the two standard orientations, have been studied via density functional theory methods (DFT). The structures investigated were constructed using, as prototypes, well-known ordered binary-alloy (AB) structures - AuCuI, Au3Cu, CuPt, "A2B2" - , in which one standard orientation corresponds to atom A and the other orientation corresponds to atom B. We show that in all the studied structures 56/56 2+2 cycloaddition polymeric bonds are formed between differently oriented molecules but not between similarly oriented molecules. It, thus, corresponds to an orientational antiferromagnetic interaction and the system can be mapped onto Ising fcc antiferromagnet [1]. The bonding type, 56/56 2+2 cycloaddition, is different from the 66/66 2+2 cycloaddition characteristic of the low-dimensional, 1D and 2D, C60 polymers, as it is formed between intramolecular single bonds of neighboring molecules and not between intramolecular double bonds.

The electronic and elastic properties of such polymeric structures were also calculated with all these 3D structures show metallic behavior [2] and the low dimensionality polymers being semiconductors.

Recently we have proposed a new, clathrate like, 3D structure of C_{60} [3]. In this structure the molecules are bounded via double 5/5 2+3 cycloaddition to all their 12 face centered cubic nearest neighbors [3]. This new bonding generates new C60 cages on the octahedral sites, equal to the original C60 molecules. On the tetrahedral sites distorted sodalite-like cages appears as a bonding consequence. The electronic and elastic properties of this polymer were also calculated with this structure having a semiconductive behavior, as the low dimensionality polymers, and higher compressibility than all the other C60 polymers.

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O8. Understanding Molecular Electrical Rectification

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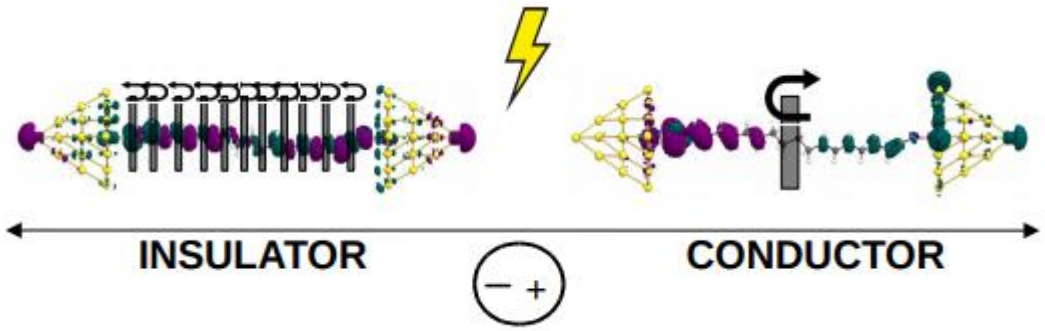
The design at nano- and molecular scale devices is one of the main goals of R&D teams within the field of electronics. The main obstacle for the development of these components at nano and molecular scale is the lack of knowledge about the physical-chemical processes that give rise to the magnetic couplings and electronic transport mechanisms. Computational simulation methods stand out as powerful tools for the analysis of the electron transport along certain material and to evaluate the effect of possible structural modifications. Herein,[1] a recently proposed method based on electron deformation orbitals is used for the study of the rectification phenomena in simple organic molecules. For this, specific experimentally and theoretically verified molecular diodes have been chosen, covering the most common design strategies. In this method, the rationalization of the electron transport in terms of the mixing of occupied and virtual orbital spaces connects directly to the band theory of conductivity in mesoscopic systems and allows understanding the rectification process from a more intuitive chemical perspective.



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O9. Nanocomposite of iron oxide and tin oxide for photocatalytic application

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Photocatalytic dye degradation is one of the important application of nanostructured metal oxide is known. In the present study, we reports the synthesis of Fe_2O_3 by auto combustion synthesis method. After it's synthesis SnO_2 was added to Fe_2O_3 nanostructure by wet impregnation methods in different weight ratios. Synthesized nanocomposite systems were well characterized using UV, FTIR, XRD and FESEM micrograph analysis. After complete characterization, Fe_2O_3:SnO_2 nanostructures were analyzed for its photocatalytic dye degradation. For photocatalytic studies two complex organic dyes (methylene blue and Crystal Violet) degradation and water splitting experiments were carried out this composites system degrade almost 70% and 60% of MB and CV, respectively within 60min. of irradiation time in natural sunlight.

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O10. Accurate prediction of COF structure from ab-initio methods

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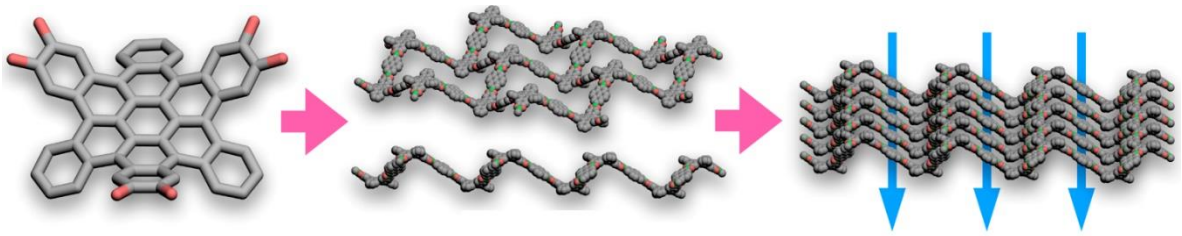
Covalent Organic Frameworks (COF) are a very active field of research, but their precise structures could be hard to determine. We employ ab-initio techniques in order to help with that task. Theoretical methods, like Tight Binding or Density Functional Theory, allow us to rank stability of possible isomers or different arrangements between layers, which also indicate porosity of the structures. Such methods, along with experimental measurements, allow insight into detailed COFs structure at different conditions.



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O11. Stability of PVP AgNPs in media of interest for polyelectrolyte multilayer build-up

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Rapid advances in the nanomaterials synthesis and characterization have enabled their safe integration into orthopaedic implants. Coating implants with metal/metal oxide nanoparticles can be considered an efficient approach to develop bioactive antimicrobial coatings that, in principle, do not promote bacterial resistance.[1] To date, various coating methods have been used, of which polyelectrolyte multilayers (PE MLs) have attracted particular attention due to the possibility of coating substrates of different size, composition, and topology. In order to obtain stable and effective PE MLs/AgNPs coatings, extensive preliminary studies of the nanoparticles' stability in various media of interest for the assembly of PE MLs are required.

The aim of this study was to find the most suitable and stable options for incorporating AgNPs into poly-L-lysine (PLL) and poly-L-glutamic acid (PGA) ML. Polyvinylpyrrolidone stabilized silver nanoparticles (PVP AgNPs) were synthesized by reduction of silver nitrate[2] and characterized by UV-Vis spectrometry and transmission electron microscopy (TEM). The stability of PVP AgNPs was investigated in ultrapure water, HEPES/NaCl buffer with or without PLL or PGA by dynamic (DLS) and electrophoretic light scattering (ELS) during 24 hours. The structure of the PLL/PGA multilayer containing PVP AgNPs was visualized by atomic force microscopy (AFM).

The PVP AgNPs had a bimodal size distribution with hydrodynamic diameters of 15.65 nm and 40.95 nm Stability studies showed that the optimal way to incorporate the NPs into the multilayer would be to adsorb a layer of NPs from a HEPES/NaCl suspension. The AFM micrographs showed that deposition of (PLL-PGA)2 (PLL-PVPAgNP) (PLL-PGA)2 ML leads to the formation of dispersed granular structures that become denser after 10 deposited bilayers i.e. [(PLL-PGA)2 (PLL-PVPAgNP) (PLL-PGA)2]2 ML, indicating successful incorporation of AgNPs.

The obtained results indicate a versatile method to prepare PE MLs containing various metal/metal oxide nanoparticles of interest for biomedical applications.

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O12. Self-cleaning SERS substrate based on ZnO nanorods and supported by Ag nanoparticles

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The purpose of this work is to demonstrate the possibility of creating self-cleaning SERS substrates based on a developed nanostructured ZnO surface using Ag nanoparticles. In this work, we used SERS substrates with the following structure (from bottom to top): Si (100) substrate with a 300 nm oxide layer; seed layer ZnO 100 nm (magnetron sputtering); array of ZnO nanorods (hydrothermal synthesis); surface layer of Ag nanoparticles (vacuum thermal evaporation + annealing). The analyte was a solution of rhodamine-B 230 μm in the form of drops of 4 μl. The samples were studied on a LabRAM HR Evolution Raman spectrometer (Horiba) with the following parameters: wavelength 514 nm; power 0.5 μW; light spot area 20 μm^2; spectrum accumulation time 50 s. The self-cleaning of the substrate occurred under the action of near UV radiation: wavelength 405 nm; light flux density 94 mW/cm^2; exposure time 120 minutes. Studies have shown that the substrates produced by SERS have a gain of 10^3. Comparison of the spectra of ZnO and ZnO/Ag substrates before and after UV treatment showed that the presence of nanoparticles increases the efficiency of photocatalytic decomposition by more than 6.5 times, making it possible to remove up to 71% of the substance from the surface substrates in the dry state. Thus, it can be argued that this design of the SERS substrate can be used repeatedly when upgrading the self-cleaning method. The work was supported by the Russian Science Foundation (Project No. 21-19-00761).

O13. Development of a SERS-active nanopipette for scanning ion-conducting microscopy

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Scanning ion-conductance microscopy (SICM) – is a method of scanning probe microscopy, where a nanosized pipette plays the role of a probe. SICM is an indispensable method in creating topography of micrometer and nanometer-sized surface. For the last decade, scientists have been trying to improve the SICM. One of the promising directions is the joint application with Surface-enhanced Raman spectroscopy (SERS). This aim is achieved by modifying the nanopipette surface with plasmonic particles. The development of a SERS-active nanopipette is an urgent task, because this solution can be used to electrically control the delivery of molecules/ions, at the same time monitoring changes in real time and measure the changes caused by the impact of the delivered molecules/ions through SERS spectra. In this case, there is practically no interaction with the object under study.

In the course of this work, we developed an approach to the formation of arrays of silver nanoparticles by vacuum thermal evaporation on the surface of a pipette. Pipettes of Borosilicate with a tip diameter of about 50–70 nm were used. To modify the surface of the pipette, arrays of nanoparticles with different average diameters were used, which ranged from 10 to 50 nm. The morphology of the resulting metal arrays of nanoparticles was studied using scanning electron microscopy. It was found that the obtained pipettes have a SERS gain comparable to commercial SERS substrates with a gain of about 10^4.
This work was supported by the State assignment 2020-2022 № FSMR-2020-0018.

O14. Formation of sensitive elements based on titanium dioxide nanowires by the direct ink writing method

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The purpose of this work is to demonstrate the possibility of forming sensitive layers of sensors based on titanium dioxide nanowires by direct ink writing. In the work, the sensitive elements of the sensors were formed on a silicon substrate with an oxide layer. TiO_2 nanowires were obtained by hydrothermal synthesis from commercial Degussa P25. To form sensitive layers using the direct ink writing method, a stand was created based on 3d printer Anet A6 with a special print head. The print head is a housing in which a glass syringe with a nozzle at the end and a mechanism is installed that allows you to controllably squeeze out the required volume of suspension onto a heated table. The nozzle can be replaced with a nozzle with a different hole diameter. The advantage of this method is the possibility of local and controlled deposition of the suspension on the substrate. The control of the stand with the help of a computer allows you to quickly change the parameters of the formation of functional layers. In the work, studies of suspensions of various compositions were carried out. The study of the resulting sensitive layers of sensors was carried out using SEM. An analysis of SEM images showed that the use of direct ink writing makes it possible to form layers with the predominant direction of TiO_2 nanowires. This feature can increase the sensitivity of the sensors. This work was financially supported by the grant of President of the Russian Federation (project МК-2201.2021.4).

O15. Chemical Synthesis of Gold Nanoparticles of Varying Shapes, Sizes, and Color for the Development of Lateral Flow Immunochromatographic Assay

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Gold nanoparticles (AuNPs) of different shapes and sizes represent significant color changes in a reaction mixture that play a promising role in the development of the rapid Lateral Flow Immunochromatographic Assays (LFIA). The present study involves the chemical synthesis of AuNPs by using various molar ratios of N-2-hydroxyethylpiperazine- N-2-ethanesulfonic acid (HEPES) and hydrogen tetrachloroaurate(III) trihydrate ($HAuCl_4$). The addition of the monosodium phosphate (NaH_2PO_4) or the disodium phosphate (Na_2HPO_4) in the reaction mixture resulted in the acceleration of the rate of reaction and the reaction completed in a few seconds with an increase in the concentration of the mono/di sodium salt. The change in the color of reaction mixtures over the period of time was recorded in terms of the absorbance of the UV-Visible light in the range of 250-750 nm of light wavelength. The particle size analysis of the nanostructures confirmed that the nano-moieties exist in the size range of 2 nm to 553 nm. The present study confirms that the change in the color of the nanostructures reactions mixtures is a function of the surface plasmon resonance bands.

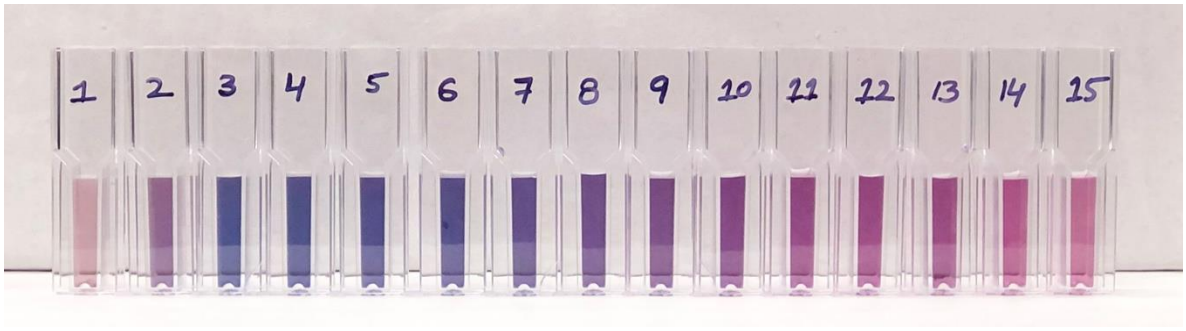

Figure 1: Change in the color of the reaction mixture with the increasing concentration of disodium phosphate.

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O16. Rapid Detection of Salmonella by using Antibody Functionalized Immuno-magnetic Iron Oxide Nanoparticles

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Rapid detection of pathogens by using functionalized nanoparticles coupled with antibodies provides advantages to detect bacterial pathogens in food and drinking water samples [1]. The study was aimed to develop an immuno-analytical assay to detect Salmonella by using magnetic iron oxide nanoparticles (IONPs) conjugated with the mouse anti-salmonella enteritidis LPS antibody. The IONPs were synthesized by reducing iron chloride and stabilized by using trisodium citrate. The morphophysical analysis of nanoparticles by using the TEM technique manifested that the nanoparticles are spherical and exist in the size range of 10-15 nm. A Williamson-Hall plot analysis of the XRD peaks gave a crystallite size of 9.9 nm. The magnetization of IONPs was recorded as 61 Am2kg-1 at 1 T by performing the vibrating-sample magnetometer analysis. Magnetic iron oxide nanoparticles were carbodiimide conjugated to mouse antibody (8209-5349) by using N-Hydroxysuccinimide (NHS) and 1-Ethyl-3-(3-dimethyl aminopropyl) carbodiimide (EDC) at room temperature [2]. Size distribution analysis of IONPs, EDC-NHS associated IONPs and carbodiimide antibody conjugated nanoparticles showed the gradual increase in the hydrodynamic diameter of IONPs after their conjugation with NHS, EDC, mouse antibodies, and finally with the bacterial pathogens. A magnet was used to sequester the Salmonella conjugated immuno-functionalized nanoparticles from water samples. Confocal microscopic images of Salmonella conjugated immuno-functionalized IONPs showed the association of immuno-magnetic nanoparticles with Salmonella. The findings of the current study confirm the potential of immuno-functionalized IONPs to separate and detect Salmonella successfully from contaminated samples.

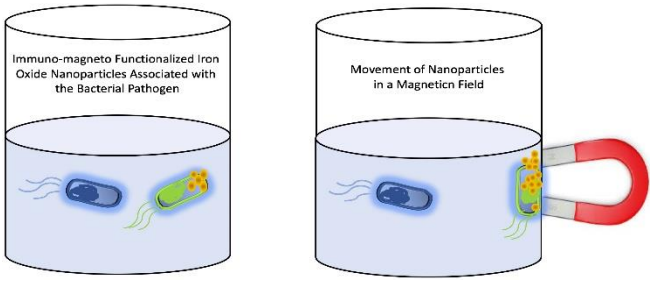

Figure 1: Movement of IONPs associated Salmonella bacterium toward a magnet.

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O17. Nanocrystalline YSZ Electrolyte by coprecipitation for Solid Oxide Fuel Cell

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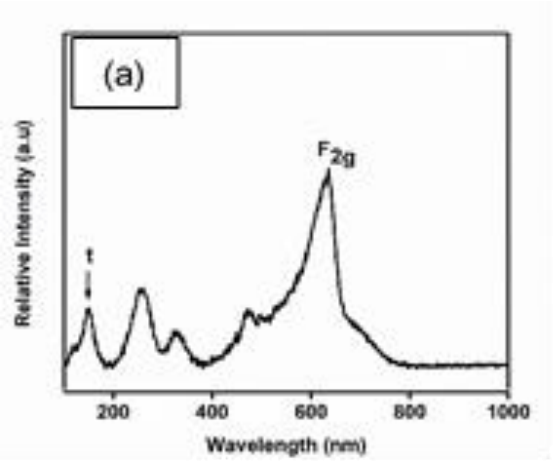
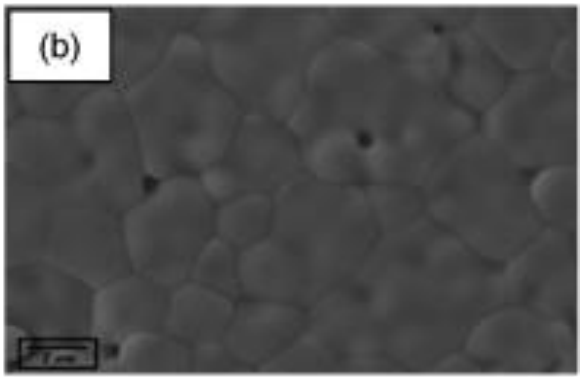
Nanocrystalline yttria stabilised zirconia (YSZ), with size crystallite size between 15 and 20 nm, were prepared by a modified co-precipitation method. The process involves the use of molecular water to facilitate the hydroxylation. Since there is no external water utilized during the precipitation process, it is expected that the as prepared and calcined materials would have minimum aggregation caused by hydrogen bonding. The synthesized materials were calcined at temperature 650°C in air and was pelletized to green body (pellet) with approximately 122MPa pressure. A density of around 95% was achieved by sintering the green body at 1450°C for around 3 hours. The calcined and pelletized YSZ samples were characterized by X-ray powder diffraction (XRD) and Raman spectroscopy for structural confirmation. Further, samples were analyzed using transmission and scanning electron microscopy (TEM and SEM). The ionic conductivity was measured by electrochemical impedance spectroscopy (EIS) of the sintered pellet in the temperature range of 650-900°C. Compared with conventional synthesis, nanopowders produced have narrow particle size distribution and better oxygen ionic conductivity, which is one of the main parameters for SOFC in order to get higher power density.





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Poster presentations

P1. Specificities of adsorption properties of nanocomposites of multiwalled carbon nanotubes and polyamide, polyethylene, polyvinyl chloride, expanded polystyrene

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The adsorption internal friction $Q^{-1}(C)$ in nanocomposites of multiwalled carbon nanotubes and polyamide, polyethylene, polyvinyl chloride, expanded polystyrene is represented partly in figure 1.

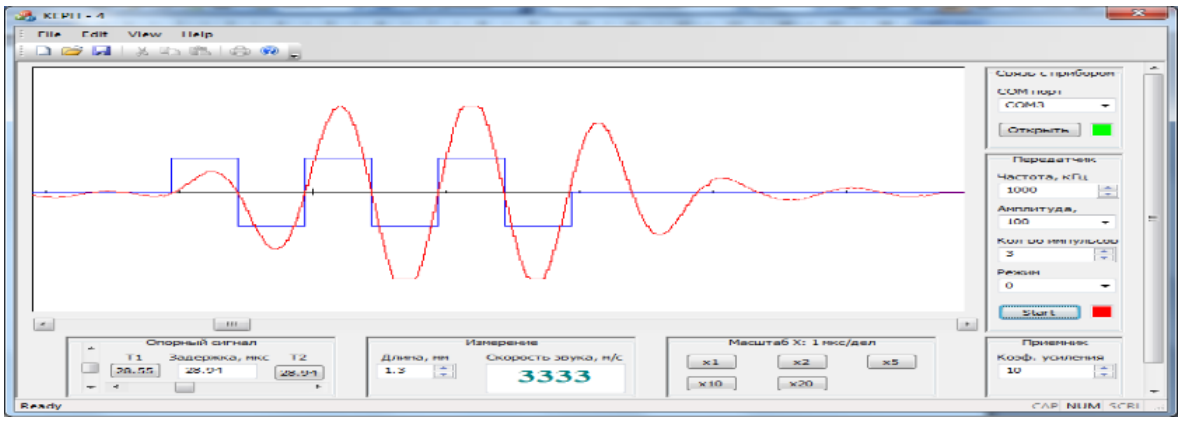

Figure 1. *The data plot illustration of the quasilongitudinal elastic waves velocity $V_{\parallel}$ = 3333 m/s in nanocomposite of polyamide + 1.7% dye blue squaring by impulse-phase ultrasonic method at frequency $f_{\parallel} \approx 1$ MHz*

Conclusion

As the result of the mechanical study the presence of a strong effect between polyamide**,** polyethylene, polyvinyl chloride and carbon nanotubes was confirmed.

Acknowledgements

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P2. Investigation of thermoelectric properties and thermal stability of low-temperature thermoelectric material based on Bi-Te-Se system

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At present, thermoelectricity is a promising area of science and technology, which is rapidly developing and shows a constant increase of interest. However, the wide practical application of thermoelectric devices is constrained by their low efficiency, which is associated with insufficient thermoelectric efficiency of thermoelectric materials (TEM) used for manufacturing these devices. One of the ways to increase the effectiveness of TEMs is nanostructuring. In this case, a significant scattering of phonons and a decrease in thermal conductivity are achieved. Another way to increase efficiency is to alloy materials and change their compositions. So, the aim of the work was to take well-known promising materials based on Bi-Te-Se and add Cl to them, since it makes it possible to obtain n-type materials. In addition, the Se concentration was changed to vary the band gap. Next, the mechanical and thermal properties of obtained materials were investigated, in particular the stability was evaluated.

An obligatory condition for the development of TEM technology is the study of their thermoelectric parameters (electrical conductivity, thermoelectric power, thermal conductivity), which makes it possible to determine the thermoelectric figure of merit. For this reason, these parameters were determined. In addition, the thermal stability of such materials is poorly investigated. So, the thermal stability of synthesized TEM was studied by simultaneous thermal cycling of samples using differential scanning calorimetry and thermogravimetry. It has been established that thermal cycling does not cause phase transitions in material. At the same time, the curves of repeated measurements are close to each other. The results of thermogravimetry show no change in the weight of the TEMs, which point out on the absence of sublimation or oxidation processes. Thus, the results of thermal cycling indicate the high stability of investigated TEM in the selected temperature ranges.

This work was supported by Russian Science Foundation (project number 21-19-00312).

P3. Investigation of the crystallization kinetics for thin films of phase change memory material $Ge_2Sb_2Te_5$

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Chalcogenide semiconductor compounds, in particular the $Ge_2Sb_2Te_5$ (GST225) material and thin films based on it, have been the objects of intensive research and development over the past decade. Due to the significant change in optical and electrical properties during phase transformations between amorphous and crystalline states, initiated by low-energy current or laser pulses, GST225 thin films have already found commercial applications in optical discs (DVD-RW, Blu-Ray) and electric phase random access memory (PCM, 3D X-Point). However, the crystallization process in GST225 thin films, which determines operation speed of phase change memory cells, is poorly understood.

In this regard, the aim of this work was to study crystallization kinetics for thin films of the GST225 material.

GST225 thin films were formed on monocrystalline silicon wafers by magnetron sputtering of a GST225 target. The thickness of the obtained films was about 1 μm. The composition was studied by Auger spectroscopy and energy dispersive X-ray spectroscopy. Structural features were determined using X-ray diffraction. Thermal properties and crystallization kinetics were investigated by differential scanning calorimetry. The measurements were carried out in aluminum crucibles at 5 different heating rates in a nitrogen flow on a DSC-50 (Shimadzu) calorimeter.

The activation energy at the beginning of crystallization is about 1.80 eV. During the reaction, it slightly decreases to 1.65 eV. It can be concluded that the crystallization mechanism does not undergo significant changes in the process of the reaction. It was shown that the crystallization kinetics is most appropriately described by the second-order model of the reaction. The dependence of the pre-exponential factor on the degree of transformation was found. Thus, the main kinetic parameters of crystallization of thin GST225 films were found.

This work was supported by a grant from the President of the Russian Federation (MK-5457.2021.4).

P4. Methods for obtaining nanostructured thermoelectric materials on the basis of Bi_2Te_3 and Sb_2Te_3 for temperature range of 200-500 K

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Thermoelectric (TE) materials on the basis of Bi_2Te_3 and Sb_2Te_3 are the most efficient for use in thermoelectric devices operating on Peltier and Seebeck effects in the temperature ranges of 200-400 and 300-500 K, respectively. One of the main ways to increase the thermoelectric figure of merit of TE materials is to obtain nanostructured materials in which the phonon component of thermal conductivity decreases. In order to obtain bulk nanostructured TE materials, the spark plasma sintering of nanodispersed powders of n-type $Bi_2Te_{2.8}Se_{0.2}$ (0.11 wt. % $Bi_{11}Se_{12}Cl_9$) and p-type $Bi_{0.5}Sb_{1.5}Te_3$ (3 wt. %Te and 0.09 wt.% Pb) were used.

A Retsch 400 PM high-energy planetary ball mill was used to obtain nanodispersed powders of TE materials. According to the developed technology, powders with a priority dispersion of 10, 20, 30 and 50 nm were obtained. Powder dispersion was studied on a scanning electron microscope FEI Helios Nanolab 650 at an accelerating voltage of 10 kV and a beam current of 0.1 nA. The bulk samples of nanostructured TE materials were obtained by spark plasma sintering using a SPS-511S at pressure of 50 MPa and temperature of 720 K for 5 minutes. The composition of powders and nanostructured TE materials were studied using a JSM-6480LV SEM equipped with INCA ENERGY Dry Cool for energy dispersive X-ray spectrometry. As a result of studies of thermoelectric parameters, the following maximum values of ZT were obtained: for $Bi_2Te_{2.8}Se_{0.2}$ (0.11 wt. % $Bi_{11}Se_{12}Cl_9$) ZT=1.15 at 360 K, for $Bi_{0.5}Sb_{1.5}Te_3$ (3 wt. %Te and 0.09 wt.% Pb) ZT=1.21 at 380 K.

P5. Thermal conductivity of nanostructured thermoelectric materials on the basis of PbTe and GeTe

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The total thermal conductivity of thermoelectric (TE) materials (κ_{tot}) is mainly determined by the phonon (κ_{ph}), electronic (κ_e) and bipolar (κ_{bp}) components. In nanostructured TE materials, phonon scattering occurs at interfaces determined by the grain surfaces. The interfaces in the material structure scatter phonons, the mean free path of which is greater than or comparable to the distance between the interfaces. The thermal conductivity has been studied in the temperature range of 300–900 K and the mechanisms of heat transfer in TE materials have been considered for n-type PbTe (0.2 wt.% and 0.3 wt.% Ni) and p-type GeTe (7.4. wt.% Bi). Nanostructured TE materials were also obtained by spark plasma sintering of nanodispersed powders with 10–50 nm sizes. The relationship of heat transfer mechanisms with the temperature dependences of electrical conductivity and Seebeck coefficient was established. For all studied TE materials, the decrease in κ_{tot} with increasing temperature in the range of 300–900 K is determined by κ_{ph}. The thermal conductivity has values at 300 K equal to 3.7 and 3.3 W/m·K for classical and bulk nanostructured PbTe, respectively, and 2.7 and 2.3 W/m·K for GeTe. Thermal conductivity has a minimum at 820-840 K, equal to 1.1 and 1.0 W/m·K for classical and bulk nanostructured PbTe, respectively, and 1.6 and 1.4 W/m·K for GeTe. Further, with an increase in temperature, κ_{tot} increases due to the appearance of bipolar heat transfer. Thus, it has been experimentally established that bulk nanostructured TE materials with similar temperature dependence have κ_{tot} values 10-12% lower in relation to κ_{tot} TE materials with a classical structure.

P6. Nanocomposite of Iron Oxide and Titanium Oxide for Photocatalytic applications

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Nanostructured metal oxides are well known for number of applications. Photocatalysis is one of the important application of metal oxide is known. Herein, we have synthesized Iron oxide by auto-combustion synthesis method. After its synthesis TiO_2 was added to Iron oxide nanostructures by ex-situ and In-situ methods in different ratios. Synthesized composite systems were characterized using UV, FTIR, XRD and FESEM analysis. After synthesis and characterization, Iron Oxide: TiO_2 nanostructures were checked for its photocatalytic behavior. For photocatalytic study two complex organic dyes (Methylene blue and Crystal violet) degradation and water splitting experiments were carried out. These composite systems degrade almost 80% and 49% of MB and CV, respectively within 90 min. of irradiation time in natural sunlight.

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P7. Influence of thin-film heat sinks and barriers on the combustion of Al-CuO_x multilayer thermites

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The main problems of micro- and nanoassemblies are how to limit and accurately dose heating, how can the heated volume be limited or how can it be localized? Energetic nanoscale multilayer thermites for surfaces bonding have been developed and partly commercialized in the past decade. Due to their high reactivity and intense heat generation, these functional foils can act as heat sources for bonding heat sensitive materials and micro- and nano-sized components.

Within the framework of this work, problem related to understanding and preventing heat dissipation in the course of a self-propagating reaction in Al-CuO_x multilayer energy materials formed on the surface of various substrates was developed and solved. To control the direction and velocity of wave combustion propagation thin-film heat sinks and barriers with a topological pattern were formed on the surface of the substrates. The formation of such accumulators and barriers, as well as multilayer thermite materials, was carried out using magnetron sputtering. The study of the combustion features of thermites and the study of their energy properties was carried out using high-speed video recording and differential scanning calorimetry, respectively.

P8. Structure and functional properties relationship in Sc-doped $LuFeO_3$

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Structural state and crystal structure of the $Lu_{1-x}Sc_xFeO_3$ ($0 \le x \le 1$) compounds prepared by a chemical route based on a modified sol-gel method and conventional two-stage solid-phase sintering have been investigated using X-ray diffraction technique and Raman spectroscopy. It was observed that chemical doping with Sc ions leads to the structural phase transition from the orthorhombic structure to the hexagonal structure via a broad two-phase concentration region of $0.1 < x < 0.45$. An increase in scandium content above 80 mol.% stabilizes the non-perovskite bixbyite phase, which is specific for compound $ScFeO_3$. The concentration stability of the different structural phases and the grain morphology are studied depending on the chemical composition and the synthesis method. The composition-dependent phase diagram has been constructed based on the data obtained by structural investigations. The comprehensive characterization of the electromechanical properties was done using laser interferometry and piezoresponse force microscopy, which revealed weak piezoelectricity in the compounds with hexagonal structure.

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P9. Photocatalytic degradation of caffeine using graphitic carbon nitride as the catalyst

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Research over the last few decades has shown that the pollutant contamination of the aquatic environment become a serious global problem. Due to the continuous and commonly ignorant release of pollutants without their prior treatment, we persistently influence the ecosystem and impact the living organisms. With this study, we present an attempt to degrade one of the pollutants, namely caffeine, with the non-toxic photocatalytic approach.

Caffeine (CAF) was dispersed in a suspension of graphitic carbon nitride (CN) nano powder, which was prepared by a simple thermal method at several treatment temperatures (at 500, 550, and 600 °C) using urea as a precursor. Synthesized CN catalysts were characterized using X-ray diffraction analysis (XRD) and photoluminescence (PL). Photocatalytic experiments were performed in an incubator under an ultraviolet A (UV-A) lamp (Supratec 18W/73, Osram) with a specified wavelength between 300 and 400 nm and a simulated solar lamp (Osram Ultra Vitalux 300W). We show that after the photo-degradation process, concentration of CAF as a model pollutant was lower compared to the initial concentration (10 mgL^{-1}). Furthermore, we also show how thermal treatment of the CN influence the photocatalytic degradation of CAF. We also noticed that the degradation is faster under simulated solar irradiation compared to UV-A irradiation. For future work, we expect that the studied photocatalyst will be reusable through immobilization, which is also of utmost significance for their implementation under real conditions.

P10. Self-cleaning SERS-active substrates using a Si-compatible process flow

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Surface enhanced Raman spectroscopy (SERS) is currently used to detect and characterize various chemical compounds in various fields of study [1]. The current SERS substrates meet the requirements for analysis well, but they are still quite expensive for routine analysis. In this regard, some efforts have been made to overcome the latter hurdle by developing reusable SERS substrates. [2]. In particular, our approach is to combine a silvered porous silicon fabricated by affordable Si-compatible process that has already proved its effectiveness as a SERS substrate [4] and photocatalytically active material (e.g. TiO_2) possessing its self-cleaning upon ultraviolet (UV) light. Si wafer was used as an initial substrate to fabricate macroporous silicon (macropor-Si) by electrochemical etching in an electrolyte. Next, the macropor-Si was coated with a TiO_2 film of 60 nm thickness by magnetron sputtering. SERS-active coating was formed by thermal evaporation of Ag nanoparticles, which diameter was about 25 nm, followed by electroless deposition of Ag dendrites. Morphological characterization of the samples was carried out with scanning electron microscope Hitachi 4800. For the SERS measurements, the obtained substrates were kept in a water solution of 10^{-6} M R6G for 2 h and then studied using 3D scanning Raman microscope Confotec NR500 equipped with 473 nm laser. The self-cleaning feature was tested in two SERS substrate with analyte. First substrate after 10 min UV irradiation, second without. After that, the Raman analysis was performed again for the both substrates, which demonstrated a pronounced cleaning the UV irradiated sample. The reported research was supported by the Russian Science Foundation (Project 21-19-00761)

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P11. Fabrication silver/hafnium oxide nanostructures on the macroporous silicon as SERS-active substrates

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At the present time there is a development of approaches in the manufacture of plasmonic materials for SERS spectroscopy which provide not only increasing of the SERS signal level from molecules, but also allow to make chemically stable, biocompatible and reusable materials. One of the approaches is the use of auxiliary oxide layers which make it possible to increases their sensitivity. Among the many oxides, hafnium oxide can be singled out, which has a high melting point and low thermal conductivity, which ensures the morphological stability of the structure [1-3]. In this work, to form a system of highly ordered pores, we used the method of electrochemical etching (anodizing) of monocrystalline silicon. The anodizing process was carried out in an electrolyte containing hydrofluoric acid and dimethyl sulfoxide at a current density of 8 mA/cm^2. Macroporous silicon was formed with diameter of pores from 500 to 1500 nm. A thin layer of hafnium oxide was deposited on the surface of macroporous silicon by the ALD method. To fabricate a plasmon coating, we used the immersion deposition of silver from an aqueous solution of $AgNO_3$ and HF. On the surface of macroporous silicon coated with a layer of hafnium oxide, silver dendrites and particles were formed. SERS-activity has been confirmed using DTNB (Ellman's Reagent (5,5-dithio-bis-(2-nitrobenzoic acid)) as analyte with a concentration of 10^{-5} M. The SERS spectra were recorded using excitation laser radiation with a wavelength of 473 nm. The research was supported by BRFFR and RFBR (projects №T21PM-136, №20-58-04016).

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P12. Formation of niobium oxide thin films by reactive magnetron sputtering

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The purpose of this work is to study the formation of thin-film structures of niobium oxide by reactive magnetron sputtering. Silicon samples with a layer of silicon oxide were used. Niobium oxide was obtained using a magnetron sputtering unit in an oxygen atmosphere. The niobium target was scattered. The main method for studying the structures was the method of Auger electron spectroscopy (AES). Samples with niobium oxide were obtained at different values of oxygen pressure in the chamber. The spectra were obtained using AES. Analysis of the spectra of the structures showed the presence of oxygen in percentage terms. Also, in some samples of niobium oxide films, oxygen not bound to niobium was found. This aroused interest in the structure from the point of view of creating memristors. Also, according to the results, it turned out that some samples have semiconductor properties. The conclusion showed that the phase transition from a semiconductor to an insulator in niobium oxide structures is observed at different pressures of oxygen supply to the vacuum-magnetron deposition chamber.

P13. Synthesis of barium titanate nanowires for a piezoelectric actuator

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The purpose of this work is to present the results on the manufacture and study of a piezoelectric actuator based on $BaTiO_3$ nanowires. The actuator is a polymer base made of PVDF, in which $BaTiO_3$ nanofilaments are dispersed. The nanofibers were obtained by a two-stage hydrothermal synthesis from commercial titanium dioxide Degussa P25. The dependence of the morphology of nanowires on the time (3, 6, 9 and 12 hours) of synthesis using SEM was obtained. The resulting nanowires were studied using Raman spectroscopy on a LabRAM HR Evolution (Horiba). To study the piezoelectric effect, $BaTiO_3$/PVDF composite samples were prepared. $BaTiO_3$ nanofilaments were dispersed in 15 ml of N,N-dimethylformamide (DMF) with stirring on a magnetic stirrer for 30 min at 1000 rpm, then 1,2 g of PVDF was added and stirring was continued until the PVDF was completely dissolved with the formation of a homogeneous and stable mixture. The mixture was then treated with ultrasonic waves for 15 minutes and stirred again for 5 minutes on a magnetic stirrer at 1000 rpm. To evaporate the solvent and create a piezoelectric film, 0.5 ml of the prepared mixture is molded into a round mold (area 7.065 cm^2, thickness: 35 μm) placed on a glass substrate and dried at 70°C for 30 minutes. Next, the film was polarized by heating it to softening and introducing needles into the film, to which voltage was applied. The study of the piezoelectric coefficient d_{33} was carried out using an atomic force microscope by the method of piezoelectric force microscopy. As a result of the work, the effect of the synthesis time of $BaTiO_3$ nanowires on their morphology, the creation of a $BaTiO_3$/PVDF composite, and the effect of different $BaTiO_3$ concentrations on the piezoelectric properties of PVDF were demonstrated.

P14. Electromechanical properties of compounds based on $BiMnO_3$

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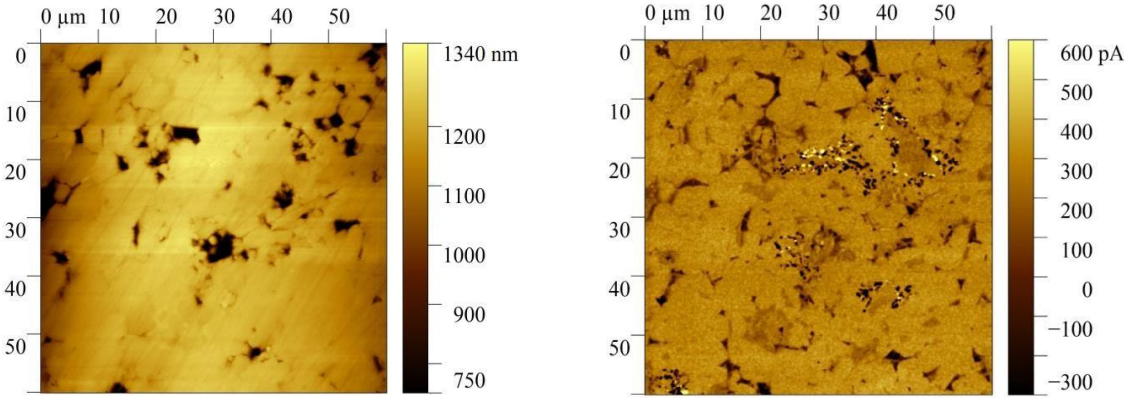
The electromechanical properties of the $BiMn_{1-x}Fe_xO_3$ compounds were studied by piezoresponse force microscopy. Images of the surface of the studied region of the compound with x = 0.2 and the corresponding piezoelectric response are shown in the Figure 1.



(a) (b)

Figure 1. Image of the surface (a) and the signal of the piezoelectric response of the compound $BiMn_{0.80}Fe_{0.20}O_3$.

It was found that the electromechanical properties of the $BiMn_{1-x}Fe_xO_3$ compounds are caused by complex domain structure, which is represented by a small number of nanosized domains. The size of the piezoactive domains ranges from 50 nm to 200 nm, and they are located extremely unevenly over the sample surface. The resulting images are characterized by high contrast, which allows to conclude that the piezosignal and the corresponding polarization are of high magnitude. The obtained data show a granular structure of the material, and a contrast from grain boundaries is found. With the help of an optical microscope, it was found that some grains left the material during the polishing process, and that it has a porous structure.

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Company presentations

SAS 3D OXIDES

Giacomo BENVENUTI

3D-Oxides, 130 rue Gustave Eiffel, F-01630 Saint-Genis-Pouilly, France

SAS 3D-Oxides is a company incorporated in December 2008, specialized in the deposition of 3D micro-patterned complex multifunctional oxide thin films materials.

For more than 10 years, 3D-Oxides have focused on R&D around the development of new complex oxide thin films materials for a wide range of applications (integrated optics, photonics, microelectronics, renewable energies, biocompatible materials and security among others). It strongly contributed to improve ABCD Sybilla equipment, expanding its facilities and improving its performances.

Among others, 3D-Oxides has been working on the development of doped or mixed (binary or ternary) oxide thin films based on titania, alumina, lithium niobate, Strontium titanate, Hafnia, Zirconia, Vanadium oxide and many more multi-element materials issued from these ones.

With a well-established experience in materials science, chemical precursors synthesis, vacuum, thin films, 3D-Oxides delivers a wide range of coated substrates to its partners/customers with combinatorial and 3D-patterned single and multi-element oxide thin films for a wide range of applications and for first functional properties tests.

ABCD TECHNOLOGY

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ABCD Technology is a Swiss company incorporated in 2006 by Dr. Giacomo Benvenuti. Since then, ABCD Technology provides R&D laboratories with its unique Sybilla equipment for oxide thin films growth.

Sybilla equipment is based on Chemical Beam Vapour Deposition (CBVD) and Chemical Beam Epitaxy (CBE) which are gas phase deposition techniques, operated under high vacuum conditions (10^{-6} mbar), in which evaporated chemical precursors are either thermally decomposed on heated substrates to form a film, or alternatively, decomposed by electrons, ions or light beams.

SYBILLA UNIQUE ASSETS

The first main asset is the possibility to achieve controlled deposition of multi-element oxide materials even on large substates (demonstrated on 450 mm).

The second asset is the combinatorial approach used to investigate rapidly materials properties and deposition process as a function of processing parameters.

The third main asset is related to additive Growth technique for oxide thin films which is a very powerful approach to achieve top level micro patterned materials during the growth both at morphological level, but also at crystalline and chemical levels. This enables totally new devices architectures.

Chemical beam vapor deposition technique with Sybilla equipment: review of main results in its 20-year anniversary

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"Sybilla" equipment has been developed for two decades to propose solutions to the challenges faced by the very promising and expanding field of oxide thin film deposition. The underlying technology named Chemical Beam Vapor Deposition (CBVD) inherits its basic concept from Chemical Beam Epitaxy (CBE) and consists in effusing (in high vacuum conditions) beams of organometallic compounds towards a substrate on which they decompose under energy activation to form the film. The technique enables deposition of multi-element oxides (up to 3 was tested, up to 5 possible), either homogenously or in combinatorial mode (i.e with controlled precursor flow gradient emitted onto the substrate, in good agreement with theoretical model predictions). High homogeneity films can be achieved, even on large substrates (scaling between 150 mm and 450 mm wafer was shown). Precursor decomposition can be initiated either thermally (substrate heating) or by irradiating with energetic beams (laser and electron activations were studied). Additive growth can be obtained by such localized irradiation, or alternatively depositing through shadow masks and benefiting from the line-of-sight nature of the technique (and exploiting the precursor decomposition kinetics not to damage masks). The multi-parameter nature of the deposition technology (precursor nature, different flows, temperature) allows to tune growth rate (from few nm/h to several μm/h) as well as thin film physico-chemical properties (chemical composition, film morphology, crystallinity, etc.) and functional properties. Combinatorial growth reveals a very efficient facility to optimize processes (in one shot, saving time and resources) and address new thin film architectures.

Notes

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