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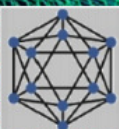
5th International Conference
“Nanotechnologies”

November 19–22, 2018, Tbilisi, Georgia

Nano–2018

Abstracts

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FOREWORD

The 5th International Conference “Nanotechnologies” (Nano – 2018) organized by the Georgian Technical University is devoted to the methods of synthesizing of nanomaterials, studying their structure, physical, chemical, and technological properties, as well as applications in techniques.

Conference will provide an evaluation of present state-of-art, new achievements, and prospects of developments in nanotechnologies. At the planned oral and poster sessions the results of experimental investigations of nanosystems will be presented, as well as theoretical approaches to their modeling.

I sure that the conference will become a forum of nanoscientists for broad interdisciplinary discussions and, therefore, not only intensify the actual collaboration, but also facilitate the future international cooperation in nanotechnology research.

Nano – 2018’s oral and poster sessions cover following fields:

- Nanotechnology
- Nanophysics
- Nanochemistry
- Nanobiology and Nanomedicine
- Nano Materials Science
- Nanoengineering and Nanoelectronics
- Nano Safety
- Nano Education

There are presented about 140 papers by authors of leading universities and research institutions from more than 20 countries.

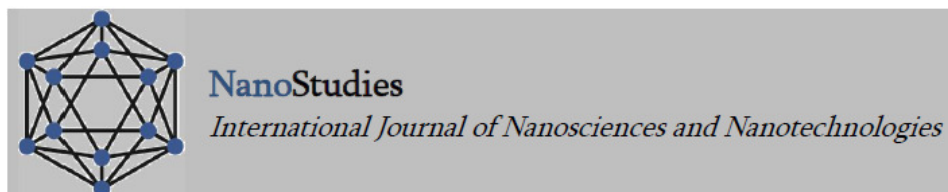
I cordially welcome participants of the 5th International Conference “Nanotechnologies”, November 19 – 22, 2018, Tbilisi, Georgia (Nano – 2018) and wish them successful and fruitful work!

Archil Prangishvili

Rector of the Georgian Technical University

Chairman of the Nano – 2018 International Scientific Committee

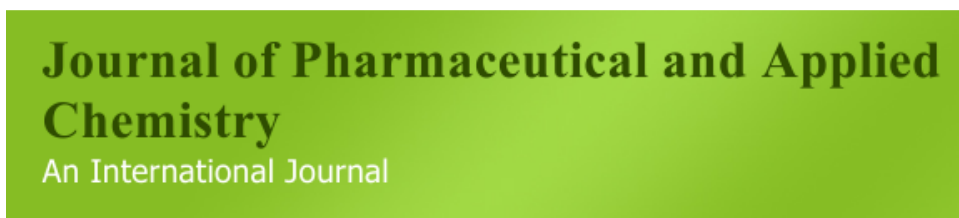
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**DIVERSITY OF MANGROVE FUNGI RECORDED
FROM SOUTH-WEST COAST OF RED SEA, EGYPT**

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Twenty-seven fungal species were collected and identified from *Avicennia marina* decayed wood from four stands located on the southern part of Red Sea coast in Egypt. Of the 27 recorded fungi, 4 species recorded for the first-time from Egypt, namely *Ascocylindrica marina*, *Eurotiumhalophilicum*, *Hortaeawerneckii*, and *Torulasp*, bringing the total number of marine fungi in Egypt to 88 species.

The highest fungal diversity was recorded at Marsa Shakraa site while the lowest was recorded at Wadi El-Jimal site. *Eutypabathurstensis* and *Stachybotryschartarum* were the most common species, while *Eurotiumhalophilicum* and *Fulvocentrumclavatisporum* were the most infrequent species. Twenty-two overlapped species were recorded between four studied sites.

Fungal communities at the three northern sites are quite different from that at southern site. Diversity of the recorded fungi compared with that recorded from tropical and subtropical mangroves. Frequency of occurrence and distribution of the recorded fungi was studied. Cluster analysis and principal component analysis (PCA) was used to compare the similarity between the fungal communities in the four studied sites.

SUCCESSIVE PHASE TRANSFORMATIONS AND TWINNING PROCESSES IN SHAPE MEMORY ALLOYS

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A series of alloy systems, shape memory alloys, exhibit a peculiar property called shape memory effect performed by the deformation in low temperature product phase condition and heating after releasing the stress.

Shape memory effect is performed by successive thermal and strain induced martensitic transformations governed by changes in the crystalline structure of material in the crystal and lattice level.

Thermally induced transformation occurs with cooperative movement of atoms occupying lattice sites in the materials on cooling from high temperature parent phase region. Thermally induced martensite occurs as lattice twinning by means of lattice invariant shear, and the twinned martensite structures turn into detwinned structures by means of stress induced martensitic transformation.

The deformed material recovers the original shape heating, and material cycles between the deformed and original shapes on cooling and heating. The microstructural mechanisms responsible for the shape memory effect are the twinning and detwinning processes as well as martensitic transformation. Martensitic transformation occurs as martensite variants with lattice invariant shears in two opposite directions, $\langle 110 \rangle$ -type directions on the $\{110\}$ -type planes of austenite matrix.

Copper based alloys exhibit this property in metastable β -phase region, which has bcc-based structures at high temperature parent phase field. Lattice invariant shear is not uniform in copper based shape memory alloys, and these types of shears gives rise to the formation of layered complex structures, depending on the stacking sequences on the close-packed planes of the ordered lattice.

In the present contribution, X-ray diffraction and transmission electron microscope studies were carried out on two copper based CuZnAl and CuAlMn alloys. These alloy samples have been heat treated for homogenization in the β -phase fields. X-ray diffraction profiles and electron diffraction patterns reveal that both alloys exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation. X-ray diffractograms taken in a long time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature. In particular, some of the successive peak pairs providing a special relation between Miller indices come close each other, and this result leads to the rearrangement of atoms in diffusive manner.

EFFECT OF BARIUM TITANATE NANOPARTICLES ON ELECTRO- OPTICAL PROPERTIES OF LIQUID CRYSTAL POLYMER

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In this study, it is found that addition of barium titanate nanoparticles will decrease the phase transition temperatures and decrease of switching times as well. The performance of the electro-optical cell has been improved and can be useful in the field of process control.

PIEZORESISTANCE OF $\text{In}_x\text{Ga}_{1-x}\text{As}$ NANOWIRES

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Semiconductor nanowires (NWs) are an ideal candidate for designing nano-sized devices utilizing mechanical and electronical degrees of freedom. Diameter of NWs could be reduced to several nanometers. Additionally, NWs could be deformed up to 5 % strain without fracture. Modulation of the electric current through NW could be implemented by changing of Schottky-barrier height between the NW and electrical contact due to piezoresistance.

Recently we have shown a unified mechanism of the surface Fermi level pinning in III-As nanowires [1]. This finding implies a fixed position of the pinning with respect to vacuum level at energy distance of ~ 4.8 eV.

It is known that in InAs the Fermi level pinning occurs in conduction band, while in GaAs it occurs in the middle of a bandgap. For $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloys with In content x of 0.9 – 0.8 realizes a flatband condition, where the pinning position equal to bottom of conduction band.

Here, we show that a tensile strain of $\text{In}_x\text{Ga}_{1-x}\text{As}$ NW with x of 0.9 – 0.8 strongly switches a rectifying contact (where a Fermi level is pinned below a conduction band) to Ohmic contact (where a Fermi level is pinned under a conduction band) and dramatically increases the NW conductivity.

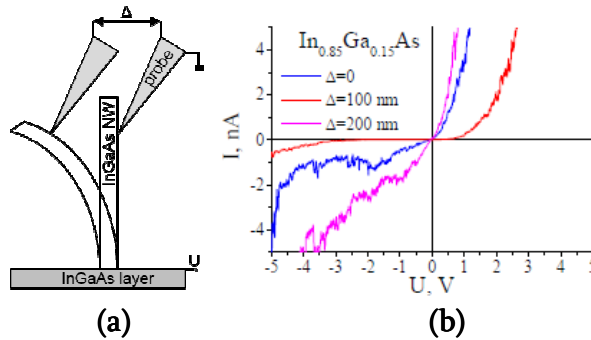


Figure 1.(a) Scheme of I – V curves measurement with simultaneous deformation of NW by SPM probe. I – V curves measured for (b) $\text{In}_{0.85}\text{Ga}_{0.15}\text{As}$ nanowires with different deformation.

Scanning probe microscopy (SPM) was used for measuring I – V curves with deforming of the NWs (**Figure 1**). By moving of the SPM probe, one can control a degree of the NW deformation by a transverse bending. It follows from the figures that for the $\text{In}_{0.85}\text{Ga}_{0.15}\text{As}$ NW the deformation leads to switching the I – V curve from rectifying to Ohmic behavior. For the 1 V bias voltage the deformation leads to a modulation of the current by three orders of magnitude.

Reference

- [1] P. A. Alekseev et al. Nanotechnol., 2018, **29**, 314003.

SILICON CARBIDE CATALYTIC SUPPORTS FOR FISCHER–TROPSCH PROCESS

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The Fischer–Tropsch (FT) technology is widely used for fuel production. Besides that, recent studies have also demonstrated the possibility to produce terminal alcohols and/or short chain olefins and C₅₊ carbons with high selectivity directly from syngas. Catalytic supports with high thermal conductivity, chemical stability and water resistivity are desirable for the FT process. The silicon carbide seems very promising for the FT catalytic supports due to processing of these set of properties.

Here we presented highly active and selective catalysts of the FT process based on electrochemically-derived porous SiC (pSiC) [1], SiC nanowires [2] (**Figure 1**) and monodispersed, 9 ± 0.4 nm, cobalt nanoparticles [3].

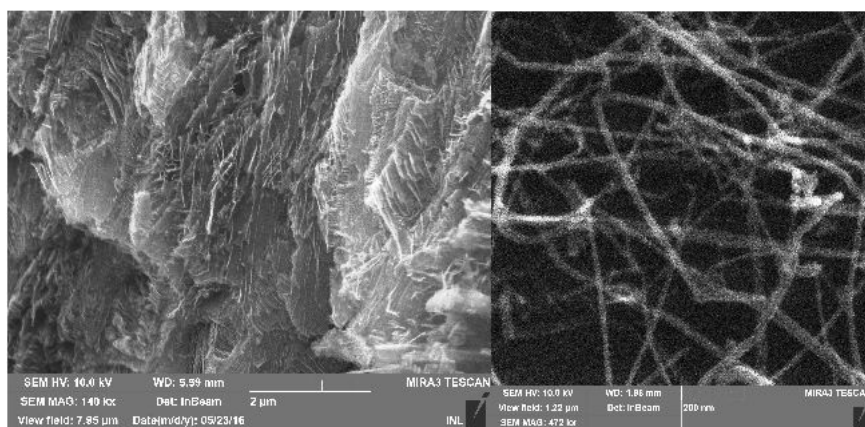


Figure 1. SEM images of porous SiC and SiC nanowires.

The catalyst based on Co/pSiC demonstrated catalytic activity in FT reaction and selectivity to C₅₊ hydrocarbons superior to Co/SiO₂ catalysts prepared by intercalation of Co NPs into commercially available Davisil SiO₂ and foam-like MCF–17 silica. The catalyst Co/SiC–NWs demonstrates reasonable overall activity, combined with unexpectedly high selectivity towards formation of C₅₊ linear alcohols.

References

- [1] ACS Appl. Nano Mater., 2018, 1, 2609–2620.
- [2] Phys. Status Solidi B, 2013, 250, 2713–2716.
- [3] Nano Lett., 2012, 12, 3091–3096.

IMPLICATIONS FOR NANO AND ADVANCED MATERIALS IN CLEAN ENERGY TECHNOLOGIES

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Nano and advanced materials offer unique properties such as optical, mechanical & electrical and play an important role in development of energy-related applications.

This presentation will discuss implications for nano and advanced materials in clean energy technologies.

It provides an overview of challenges in the manufacturing, formulation and scale up. Case studies and examples will be given and the state of the art will be discussed.

NEW ENERGETIC MATERIALS BASED ON GRAPHENE–METAL NANOPARTICLES

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Metal-organic frameworks (MOFs) attract a lot of interest as potential energy materials, because of their high density and high heat of detonation. The porous crystalline structure attracts attention due to its high specific surface characteristics and the possibility of changing their physicochemical properties by introducing metal centers. A method for synthesizing multilayer graphene-metal frameworks (GMFs) from vegetable wastes such as rice husks or walnut shells has been developed.

The use of graphene-metal structures as energy-intensive additives can become one of the promising ways to improve the efficiency of high-energy rocket fuels. It is determined that graphene oxide structures with a high specific surface and developed texture characteristics with an additive of 1 % are effective initiators of the thermal decomposition of hydroxylammonium nitrate and are capable of reducing the temperature of the onset of decomposition of the substance to a value in the range of 40 to 100 °C, as well as to decrease the activation energy from 110 ± 5 to 85 ± 9 kJ / mol. It has been established that graphene oxide structures, depending on the concentration of 1 – 5 % of the total mass, promote the convective burning rate of hydroxylammonium nitrate. An increase in the linear combustion speed of hydroxylammonium nitrate to 400 mm / s (initial pressure of 6 MPa) and the ability to reduce the required initial pressure to 1 MPa are established to provide self-sustaining combustion conditions with the addition of GOFs based on rice husks (1 % of the total mass).

Based on experimental results, it was found that the addition of 1 % GOFs affects the rate of evaporation of water droplets and methanol in the form of a reduction in the evaporation time of droplets for both liquids by 30 % and a decrease in the boiling point of the liquids. On the basis of these data, it is possible to develop a method for purifying sewage from various toxic metal salts that precipitate.

ON SOME CONDENSED PHOSPHATES OF MONO- AND POLYVALENT METALS AND SPHERES OF THEIR APPLICATIONS

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Condensed phosphates of polyvalent metals are foreordained to play a great role in our “high-tech” society in the coming decades. This conclusion is founded upon the tendency of increasing applications resulting from the electronic arrangements of these materials that based to their exceptional physical, magnetic, optical, electrical and chemical properties so flexible to the demands now being positioned on materials [1 – 3].

Many innovative and original studies in the field of condensed phosphate’s chemistry have begun in the 19th c. In the 20th c. more serious attention of researchers was dedicated as well to the chemistry of double condensed phosphates of polyvalent metals. This field of inorganic polymers developed much rapidly due to the evolution of methods of analysis and the importance of considerable application of phosphate materials in several domains. Mentioned condensed phosphates, in fact the inorganic polymers are used as raw components for manufacture of phosphates glasses; the application of crystalline and non-crystalline ultra-phosphates in quantum electronics are caused by their structure and specific features such as the thermal, vibrational and luminescent properties.

The other spheres of application of condensed phosphates are: thermo-resistant materials, effective applying fertilizers, detergents, cement substances, ion-exchange and catalytic agents, bio-materials.

The use of the phosphates is known in fine arts also (thermo phosphate painting – “Thermo Phosphate Pictorial Art” developed by O. Pavlov) [4].

Thereby application of phosphates is so large and the further investigations in this branch of inorganic chemistry must be interesting for scientists, especially in purpose to enlarge the sphere of utilization of condensed compounds [5].

References

- [1] A. Oudahmane, D. Avignant, D. Zambon. Dipotassium dialuminium cycloocta-phosphate. *Acta Crystallogr. E*, 2010, 66, 7, i49-i50.
- [2] M. A. Avaliani, I. V. Tananaev, M. K. Gvelesiani. synthesis and investigation of double condensed phosphates of scandium and alkali metals. In: *Phosphorus, Sulfur, Silicon & Rel. Elements*, 1990, 51, 1-4, 453-453.
- [3] N. N. Chudinova, I. V. Tananaev, M. A. Avaliani. Synthesis of gallium–potassium binary polyphosphates in polyphosphorous acid melts. *Inorg. Mater.*, 1977, 13, 12, 2234-2235.
- [4] I. V. Tananaev, X. Grunze, N. N. Chudinova. Prior directions and results in the domain of condensed phosphates’ chemistry. *Inorg. Mater.*, 1984, 20, 6, 887-900.
- [5] M. Avaliani. New inorganic polymers-condensed phosphates obtained in multi-component systems from solution-melts of phosphoric acids. *Nano Studies*, 2016, 13, 135-138.

AREAS OF CRYSTALLIZATION OF CONDENSED SCANDIUM AND SYLVER PHOSPHATES AND REGULARITIES OF THEIR FORMATION

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Development of nano-technologies for obtaining of inorganic polymers, notably double condensed phosphates of polyvalent metals, as well as research of areas of their crystallization, are very important [1, 2].

Table 1. Reliance of composition from temperature T and molar ratio

$n = \text{AgO}/\text{Sc}_2\text{O}_3$. \diamond – $\text{Sc}(\text{PO}_3)_3\text{-C}$, \circ – $\text{Sc}(\text{PO}_3)_3\text{-C}^{\text{I}}$, Δ – $\text{AgScHP}_3\text{O}_{10}$,
 \odot – $\text{AgScP}_4\text{O}_{12}$, \square – $\text{AgSc}(\text{H}_2\text{P}_2\text{O}_7)_2$, \blacksquare – AgScP_2O_7 , and \blacktriangle – $\text{Ag}_2\text{ScP}_3\text{O}_{10}$.

$T, ^\circ\text{C}$	$n = 1.5 - 2.5$	$n = 3.5 - 5.0$	$n = 6.0 - 7.5$	$n = 8.0 - 10.0$
130 – 150	\diamond	Δ	\square	\square
180 – 200	\diamond	Δ	Δ	Δ
220 – 240	\diamond	\odot	\odot	\odot
310 – 355	\circ	\odot	$\odot \Delta$	\odot
400 – 450	\circ	Δ	Δ	\blacktriangle
500 – 550	\circ	Δ	Δ	\blacksquare

Presented work is the outcomes of synthesis and estimation of areas of crystallization of double condensed phosphates of some trivalent and monovalent metals in correlation with temperature & molar ratio of initial components. Many double condensed compounds are obtained at temperature range 100 – 600 °C. More interesting synthesized inorganic oligomers and polymers are presented in the **Table 1**.

References

- [1] M. A. Avaliani, I. V. Tananaev, M. K. Gvelesiani. synthesis and investigation of double condensed phosphates of scandium and alkali metals. In: Phosphorus, Sulfur, Silicon & Rel. Elements, 1990, 51, 1-4, 453-453.
- [2] N. N. Chudinova, I. V. Tananaev, M. A. Avaliani. Synthesis of gallium–potassium binary polyphosphates in polyphosphorous acid melts. Inorg. Mater., 1977, 13, 12, 2234-2235.

RADIATION INDUCED NONLINEAR CROSS SECTIONS OF CONDUCTIVE ELECTRONS SCATTERING ON CHARGED IMPURITIES IN BILAYER GRAPHENE

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Graphene and multi-layer graphene films have engaged a huge interest because of their unique physical properties [1]. Many important physical phenomena that unite low-energy physics of condensed matter and quantum electrodynamics were investigated in a monolayer of graphene [2]. Bilayer graphene (AB stacked) is also of great interest since its electronic states are considerably richer than those of monolayer graphene, and multiphoton resonant excitations and high-harmonic generation in bilayer graphene were considered in [3]. The energy range of interest lies in the THz domain, where high-power THz generators and frequency multipliers are of special interest, and in general, the role of THz radiation for the study of nonlinear phenomena in condensed matter physics is important. The relativistic quantum theory of induced scattering of 2D Dirac particle on an arbitrary electrostatic field of impurity ion in the presence of an external electromagnetic radiation field (actually terahertz radiation to exclude the valence electrons excitations at high Fermi energies) has been developed [4, 5].

In the presented work, the quantum theory of nonlinear stimulated scattering of charged carriers on the Coulomb field of impurity ions in the presence of an external strong coherent electromagnetic radiation in doped bilayer graphene is developed. The interaction of electrons with the scattering potential is considered in the Born approximation. The analytic formulas in case of screened Coulomb potential have been analyzed numerically for actual parameters of interaction system in the strong radiation field. The results of our investigations show that in the THz domain of frequencies one can achieve efficient rates of absorption of pump waves of moderate intensities by this mechanism.

This work was supported by the RA MES State Committee of Science and Belarusian Republican Foundation for Fundamental Research (RB) in the frames of the joint research projects SCSAB16–19 and BRFFR F17ARM–25, accordingly.

References

- [1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov. *Science*, 2004, 306, 666.
- [2] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, A. A. Firsov. *Nature*, 2005, 438, 197.
- [3] H. K. Avetissian, G. F. Mkrtchian, K. G. Batrakov, S. A. Maksimenko, A. Hoffmann. *Phys. Rev. B*, 2013, 88, 165411.
- [4] A. K. Avetissian, A. G. Ghazaryan, Kh. V. Sedrakian, B. R. Avchyan. *J. Nanophoton.*, 2017, 11, 036004.
- [5] A. K. Avetissian, A. G. Ghazaryan, Kh. V. Sedrakian, B. R. Avchyan. *J. Nanophoton.*, 2018, 12, 016006.

NOVEL TWO DIMENSIONAL NANOSTRUCTURES AS POTENTIAL ACTIVE MEDIA FOR HIGH HARMONIC GENERATION

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In the last decade, graphene and its analogs – silicene, germanene, and stanene have attracted enormous interest due to their unique electronic and optical properties. The novel 2D nanostructures as potential effective optical materials have triggered many nonlinear optical studies. In particular, graphene-like nanostructures can serve as potential active media for nanolasers and frequency multipliers. Depending on the nanostructure symmetry the odd- and even-order nonlinear optical effects can occur. In particular, freestanding graphene is centrosymmetric and even-order nonlinear effects vanish within the dipole approximation. With the breaking of the inversion symmetry in these nanostructures, one can also observe even-order nonlinear optical effects.

With the increase of the pump wave intensity, one can enter into the regime [1, 2] where multiphoton effects are essential and high-harmonics are generated [3], which until the last decade have been the prerogative of atomic systems. Hence, it is of interest to investigate the potential of these nanostructures as an active medium for high harmonic generation process.

In the presented work, we develop a nonlinear microscopic theory of interaction of a 2D nanostructure with the coherent electromagnetic radiation taking into account the electron-electron Coulomb interaction using the self-consistent Hartree-Fock approximation. The carrier-carrier and carrier-phonon scattering processes are described phenomenologically. With the solution of the derived equations for the density matrix, we investigate the high harmonic generation process in 2D nanostructures depending on the pump field polarization, relaxation processes and the many-body Coulomb interaction between the charge carriers. Our results show that novel graphene-like nanostructures can serve as an effective medium for the high harmonic generation in the wide range of pump frequencies.

References

- [1] H. K. Avetissian, A. K. Avetissian, G. F. Mkrtchian, Kh. V. Sedrakian. Phys. Rev. B, 2012, 85, 115443.
- [2] H. K. Avetissian, G. F. Mkrtchian, K. G. Batrakov, S. A. Maksimenko, A. Hoffmann. Phys. Rev. B, 2013, 88, 165411.
- [3] N. Yoshikawa, T. Tamaya, K. Tanaka. Science, 2017, 356, 736.

THERMODYNAMIC ANALYSIS OF INTERACTION OF CARBON WITH TiO_2 , ZrO_2 , AND B_2O_3 AND OBTAINING MIXTURE OF BORIDES AND CARBIDES OF TITANIUM AND ZIRCONIUM

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At this stage of development of the industry, composite nanostructure materials are widely used. Among them it should especially be noted materials containing carbides and borides of metals TiB_2/TiC and ZrB_2/ZrC . Borides and carbides of titanium and zirconium have a unique set of physical and chemical properties (high hardness, high-temperature strength, corrosion resistance, radiation and wear resistance).

In the literature, different methods of obtaining of these compounds are known and their use becomes to be more promising.

The innovation of presented work is studying of physical and chemical bases of high-temperature processes of receiving carbides and borides of the specified systems that will give the chance of carrying out the minimum quantity of experiments.

Therefore, in the work presented by us, the task of carrying out the thermodynamic analysis of FTA (full thermodynamic analysis) [1] of the process for the production of carbides and borides of titanium and zirconium (Ti-B-O-C and Zr-B-O-C) was performed, and, based on it, the analysis of carrying out experimental studies on obtaining nanostructured compositional materials.

Data on FTA of the considered system in literature aren't found by us. Therefore the great interest represents its reception for the specified system. Calculations are carried out on the computer with application of the ASTRA-4 program described in Ref. [1]. They are performed in the temperature range 500 – 2000 K with a step of 50 ° in vacuum.

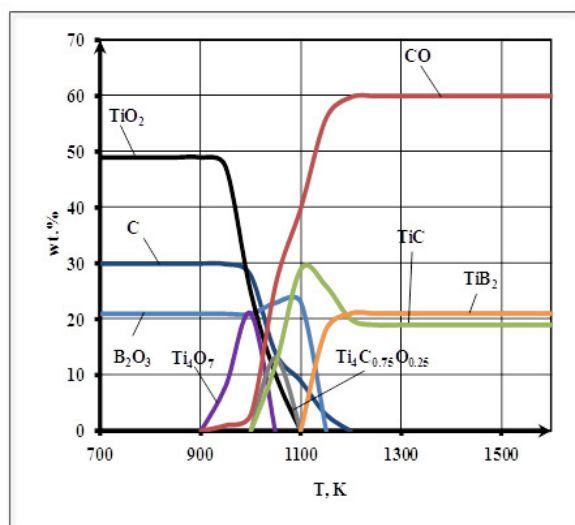


Figure 1. Dependence of components content on temperature for reaction (1) in vacuum.

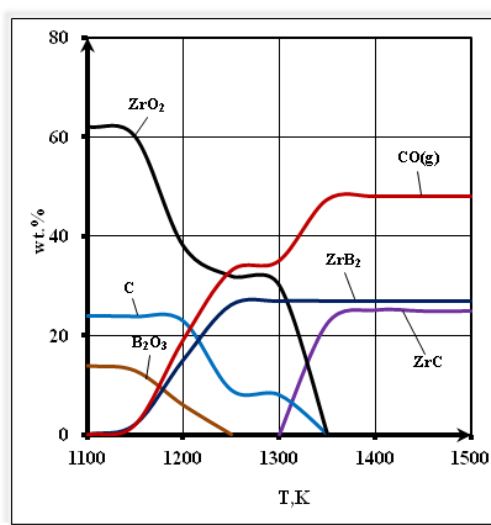


Figure 2. Dependence of components content on temperature for reaction (2) in vacuum.

The full thermodynamic analysis (FTA) of the systems Ti–B–O–C and Zr–B–O–C in vacuum was carried out for the following reactions:



and



The main results of FTA for both compositions are presented in the form of diagrams (**Figures 1 and 2**).

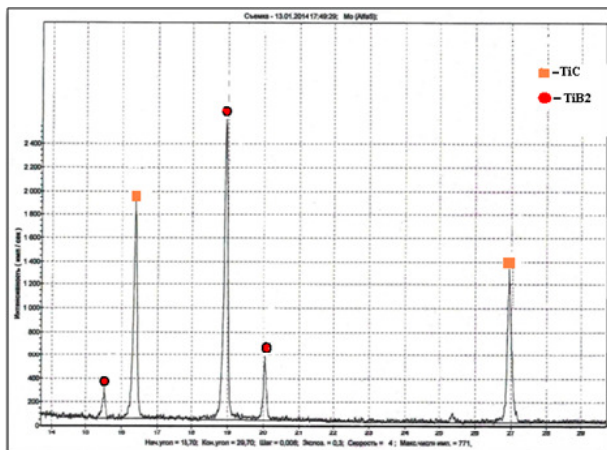


Figure 3. XRD diagram of TiB₂ and TiC mixture.

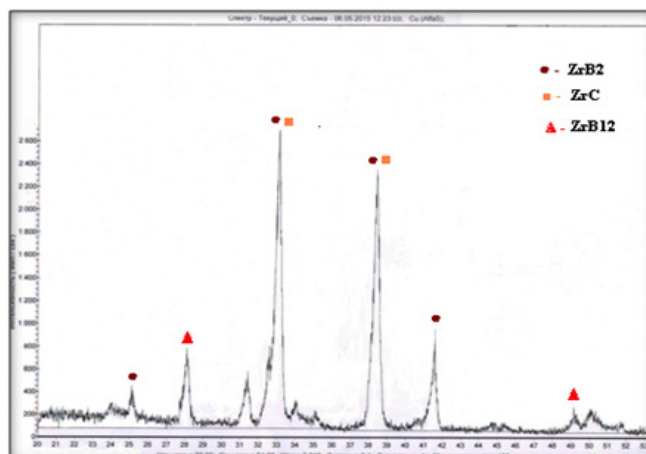


Figure 4. XRD diagram of ZrB₂ and ZrC mixture.

The X-ray diffraction patterns of the powders obtained are presented in **Figures 3 and 4**.

In conclusion, one can state that:

1. Full thermodynamic analysis (FTA) of the Ti–B–O–C and Zr–B–O–C systems was carried out in the temperature range of 500 – 2000 K in vacuum, and based on this analysis, experimental studies were carried out to obtain TiB₂/TiC and ZrB₂/ZrC composite materials.
2. X-ray diffraction patterns of the obtained powders indicate that generally it turns out mixes TiB₂/TiC and ZrB₂/ZrC.

Reference

- [1] N. A. Vatolin, G. K. Moiseev, B. G. Trusov. Thermodynamic Modeling in High-Temperature Inorganic Systems, 1994, Moscow. Metallurgy, 352 pp.

MAGNETOTHERMOPOWER OF FERROMAGNETIC Co/Al₂O₃ AND Co/SiO₂ NANOCOMPOSITE FILM AND QUASIEXCITON INSULATOR

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The effect of the magnetic field H on thermopower (TP) in films of ferromagnetic nanocomposites (FMNC) with nanoparticles (NP) Co in Al₂O₃ and SiO₂ matrices was studied. The result was estimated as the coefficient of magneto-TP – δ_α .

For FMNC Co/Al₂O₃, the value of $\delta_\alpha > 0$ exceeds the value of $\approx 70\%$ [1]. For Co/SiO₂, δ_α is negative and reaches $\approx -90\%$. The concentration of Co did not exceed the percolation threshold values. Such sharp difference of magnetic characteristics of the NC can be explained by the features of the composition and magnetic properties of the NP.

Hopping conductivity in NC occurs due to vacancies of oxygen in the matrix and NP. In the Al₂O₃ matrix, the magnetic moments of the NP and free electron spins in the external field H are collinear [1]. This leads to their mutual “repulsion” in the process a transport and substantially reduces the number of scattering NP’s. The consequence of this is an increase in the conductivity of the films and their α_H , which reaches a giant value of ~ 0.01 V / K [1].

The FMNC consisting of Co in an oxygen-containing matrix is covered with CoO [2]. In the SiO₂ matrix, $\delta_\alpha < 0$ is a consequence of the interaction of electron spins and positively charged magnetic oxygen vacancies (OV) with the Co–CoO interface [3], stimulated by the magnetic field. Spins and magnetic moments of OV are antiparallel in an external magnetic field, which leads not only to the Coulomb, but also to the magnetic attraction of electrons and OV. As a result, the electron “sticks” to the OV, a state arises that excludes electrons from transport processes due to the small mobility of the OV. Such a state can be considered as quasi-exciton dielectric (QED). The QED lifetime is probably not large, but this leads to an increase in the resistance of the FMNC and a significant negative value of δ_α .

In Co/Al₂O₃ QED does not arise due to a large dielectric constant (Al₂O₃ – $\varepsilon = 10$ and SiO₂ – $\varepsilon = 3.9$). The degradation of the magneto-TP over time indicates the significant role of the OV.

References

- [1] G. V. Lashkarev, M. V. Radchenko, M. E. Bugaiova, V. Knoff, T. Story, Y. A. Stelmakh, L. A. Krushinskaya, M. Foltyn, A. I. Dmitriev. <https://doi.org/10.1002/pssb.201700153>.
- [2] G. V. Lashkarev, M. V. Radchenko, M. E. Bugaiova, V. Knoff, T. Story, Y.A. Stelmakh, L. A. Krushinskaya, V. I. Sichkovsky, A. I. Dmitriev. *Low Temp. Phys.*, 2013, 39, 66.
- [3] A. Morozovska, E. Eliseev, M. Glinchuk. *Phys. B*, 2011, 15, 1673.

SYNTHESIS OF GRAPHENE OXIDE FROM INDUSTRIAL WASTES

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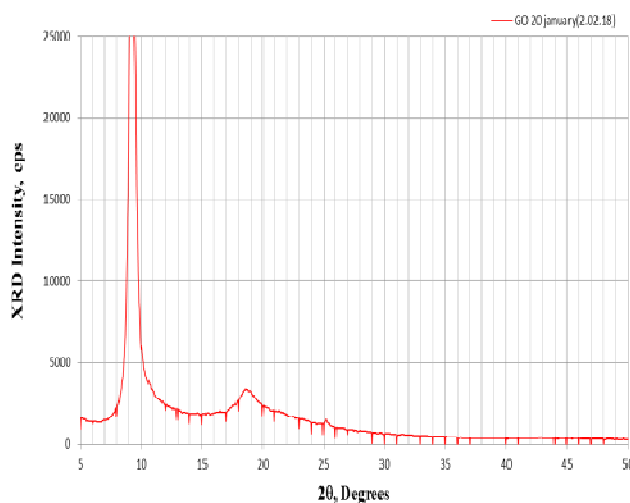
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We have synthesized graphite oxide (GO) and reduced graphene oxide (rGO) from industrial wastes – graphite foils. Flexible graphite foil (FGF) is widely used in chemical, petrochemical, metallurgical processes, for the production of ceramic composites. It is characterized by inert and anticorrosive properties and is an ideal thermal insulation material for high-temperature processes, etc. Different sizes of foil pieces (FGF) remaining from different technological processes were used for obtaining GO and rGO (**Figure 1**).



I



II

Figure 1. Image of the wastes (I) and XRD samples of GO (II) obtained from them.

Practically they are expanded graphites, and their chemical oxidation can be done using known methods with some adjustment. First of all, dry or wet grinding of wastes, removal of various types of impurities and sifting is necessary. The following oxidative systems were used to oxidize the obtained expanded graphite powder: $\text{NaNO}_3\text{--KMnO}_4\text{--H}_2\text{SO}_4$, $\text{KMnO}_4\text{--H}_2\text{SO}_4\text{--H}_3\text{PO}_4$, and $\text{KMnO}_4\text{--H}_2\text{SO}_4$.

Depending on the oxidative system, the reaction was carried out under different conditions (0 – 50 °C for 2 – 10 h). Hydrogen peroxide solution was used for the decomposition of the reaction mixture. It was confirmed that, in contrast to graphite powder, the oxidation of a powder of the same size obtained from waste requires 20 – 25 % more sulfuric acid.

ON ORIGIN OF BORON DEPOSITS

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Boron B (together with lithium Li and beryllium Be) belongs to the least abundant chemical elements. Explanation can be found in cosmology: in order to synthesize boron nuclei, Nature requires an environment that is dramatically different from those producing the remainder of the Periodic Table.

Role of boron in forming of molecular, nano-, and solid state structures is incommensurably great. Understanding of the structural diversity of boron-containing materials reduces to the electronic structure of B atom in isolated state. Configuration of valence electrons peculiar to the free B atom, $2s^2 2p$, in bounded structures becomes energetically unstable and tends first to $2s^2 2p^2$ and then even to $2s^2 2p^3$ by adding electrons from foreign atoms and / or defects usually in high concentrations peculiar to boron-rich structures. Because all-boron structural units are highly electron-deficient, elemental boron crystalline and amorphous modifications as well as boron-rich solids exhibit very complex atomic structures. Diversity of atomic and, consequently, electronic structures and related properties of boron-rich materials yields extremely wide field for their industrial applications.

In the current literature, there is stated that deposits of borate minerals found on the Earth usually are located in arid desert regions with a geological history of volcanic and / or hydrothermal activity. However, assumption on their geological origin contradicts the well-established fact that boron deposits are extremely rare and mainly concentrated in relatively small region (72 %, in Turkey). It is an argument supporting theory of cosmological origin of boron deposits on the Earth.

Some further speculations on origin of boron deposits will be presented.

CRITICAL CURRENT IN STRIP BASED ON JOSEPHSON MEDIUM

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Based on averaging the parameters of individual Josephson junctions (applying the London model for each transition), a material equation was obtained that relates the average current density \bar{j} in the medium and the vector potential of the magnetic field \bar{A} [1]: $\bar{j} = -(\bar{A}c/4\pi\lambda^2)\exp\left[-(\pi/16)(2\pi Aa/\Phi_0)^2\right]$, where $\Phi_0 = hc/2e = 2.07 \cdot 10^{-15}$ T · m² is the magnetic flux quantum of, a is the average distance between centers of granules forming the Josephson junction, λ is the penetration depth of the (exponential) weak magnetic field into the medium under consideration. The value λ is determined by the “microscopic” parameters of the medium—the average values of the distance between the centers of the granules, the density of the Josephson junctions in the medium, and the critical current of the transitions. Based on above relation, the flow of a constant electric current through a strip wire from a Josephson medium (a granular superconductor) from a different configuration is simulated. It is shown that, for strip wires, the transport current is concentrated in a narrow near-boundary region of $2 - 3 \lambda$ thickness, and in the central part of the wire the current density is much smaller. A strong non-uniform distribution of the transport current along the conductor cross-section is realized when the linear dimensions of its cross-section (thickness or width) exceed the value λ many times. This leads to a nonlinear dependence of the critical current on the geometric dimensions of the conductor. Thus, the critical current density decreases with increasing thickness and width of the strip conductor. In the other case, when the linear dimensions of the conductor cross section are much less than λ the critical current density, the practical value does not depend on the geometric dimensions of the conductor. Thus, when one strives to attain as much as possible the value of the transport current through wires from the Josephson medium, it is advisable to make them in the form of a “lithcendrat”, that is, consisting of a large number of separate strip veins with dimensions of not more than a few, isolated among themselves. We note that the values in the Josephson medium can have dimensions of the micron and sub-millimeter values, which is several orders of magnitude higher than similar values in the traditional superconductor. Consequently, it is much easier to realize a “lithcendrate” from a granular superconductor or ceramic high-temperature superconductor than from a traditional superconductor.

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Reference

- [1] M. V. Belodedov, L. P. Ichkitidze. J. Eng.: Sci. & Innov., 2013, 10, 22. DOI: 10.18698/2308-6033-2013-10-1094.

SOFT X-RAY PHOTOEMISSION STUDY OF Cs ADSORPTION ON InN AND GaN SURFACES

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The III-nitrides, namely, InN, GaN, and AlN have revolutionized solid state lighting and continue to attract substantial research interest due to their unique properties and importance for optoelectronic devices that cover a wide spectral range from the infrared to the ultraviolet. The GaN and InN-based hetero-structures are also important elements in modern high power high frequency electronics. The technical applications in micro and nanoelectronics require a comprehensive knowledge of the structural and electronic properties of both the InN–GaN volume and surfaces. Data present first photoemission results obtained for the Cs ultrathin layer adsorbed on the InN and GaN surfaces and shown possibility of photoemission method to study effect of Cs adsorption on the electronic properties of these III-nitrides. We perform first photoelectron spectroscopy (PES) study of electronic structure of the ultrathin Cs/InN and Cs/GaN interfaces. Experiments were carried out *in situ* at BESSY II synchrotron, Berlin, using PES with photon energies in the range of 80 – 900 eV. The normal photoemission spectra from the valence band (VB) and In 4*d*, N 1*s*, Ga 3*d*, Cs 4*d* core levels have been revealed under different cesium coverage.

The intrinsic surface states for the clean GaN surface at binding energies of ~ 5 and 7 eV are attenuated during Cs adsorption. Simultaneously three Cs induced surface states are found to arise. Drastic changes in the surface state spectrum were ascertained and shown to be originated from the local interacting Ga dangling bonds and adsorbed Cs atoms initiating the electron redistribution effect with formation of the semiconductor-like Cs/n-GaN interface. The surface and interface are identified as semiconducting-like and the band bending caused by the Cs adsorption is detected. The modification of the surface state spectra is evident to originate from the interaction between Cs adatoms and Ga dangling bonds that leads to hybridization among Ga 4*s* – 4*p* and Cs 5*p* – 6*s* orbitals. The Cs adsorption is found to induce the negative energy shift of the Ga 3*d* core level spectrum that is originated from the charge transfer from Cs adatoms to Ga surface atoms with increasing the Ga-valency. For the Cs/InN interface, the In 4*d* peak displays the strong core level shift and the appearance of an additional In 4*d* peak originated from In–Cs bonding. Change in the surface electronic structure of the InN caused by Cs adsorption is found to originate predominantly from suppression of the intrinsic surface state concerned with the local interaction between In dangling bonds and Cs adatoms.

Authors thank synchrotron BESSY II and Russian–German Beamline, Helmholtz Zentrum, Berlin, for providing facilities to perform experiments and help during experiments.

INNOVATIVE MAGNETRON ION-PLASMA ELECTRODISPERSION EQUIPMENT FOR SYNTHESIZING METALLIC NANOPOWDERS

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Methods for making metal's nanopowders largely determine their activity. The physical methods of producing nanopowders are mainly based on evaporation in vacuum, rapid cooling and condensing of metals. In this case, high rates of cooling speed are one of the prerequisites for receiving active nanopowders. The method of electrodispersing of liquid-phase droplets is widely used in modern nanostructure technologies; it is based on the Rayleigh (capillary) instability. Due to that, if the droplet charge of R radius reaches the critical value

$$Q_c = 8 \pi (\epsilon_0 \alpha R^3)^{1/2},$$

the process of droplet distribution begins; here α is a surface tension coefficient [1]. The droplets formed during emission process are also unsustainable, and we obtain the cascade decaying of droplets to the sizes

$$d_{\min} \approx 8 \cdot 10^{-7} \epsilon_0 \alpha^{-3}.$$

At this size, the particles lose charge as a result of the electronic emission. For the majority of materials, these sizes comprise several nanometers and are distributed in a narrow range. Therefore, the methods of electrodispersing are very promising to obtain high-dispersed materials.

In the 80s of the last century, we created the planar magnetron sputtering device. It is original construction and represents new generation of magnetrons with a rotating magnetic field. The flow of refrigerant fluid flows with high turbulence in the system and used for the rotation of magnetic unit in the cathode node [2]. The refrigerant fluid flow falls with pressure on the holding blade of the magnetic system and triggers the rotation of the entire magnetic block. The rotation of the magnetic system, which is under the sputtering disc cathode-pellet in its immediate vicinity, ensures the synchronous rotation of the magnets, which are distributed along the closed contour under cathode surface. The configuration of the magnetic system derived mathematically by us, provides formation of the even erosion on the target surface.

To date, we have developed a new and innovative magnetron ion-plasma electrodispersion device and the method of nanostructure production [3, 4]. The magnetron ion-plasma electrodispersing device and the vacuum equipment will provide the effective transition of the cathode-pellet material to nanostructures and receiving of metallic

nanopowders of high purity. The equipment may be used to receiving highly active nanopowders, which also makes it useful in fundamental research and practical application.

References

- [1] A. I. Grigor'ev, S. O. Shiryaev. Regularities of Rayleigh disintegration of charged drop. J. Tech. Phys., 1991, 61, 3, 19.
- [2] Z. V. Berishvili, I. I. Gadakhabadze, I. I. Kordzaxia, G. G. Dekanozishvili. Planar magnetron sputtering Device: A new generation of magnetron sputtering design and technology. J. Phys. Sci. & Appl., 2017, 7, 5, 28-39.
- [3] Z. Berishvili. Planar Magnetron Sputtering Device. GE P 2016 6512 B, 2015.05.28, Date of Publication: 2016.03.25 № .
WIPO|PCT, WO 2016/189337 A1, Date of Publication № WO 2016/189337 01.12.2016.
Application of India Patent, № 201717040689, November 14, 2017.
- [4] Z. V. Berishvili. The method of obtaining nanomaterials in vacuum and the magnetron sputtering device for its implementation. Application of Georgia Patent, № AP 2018 14793, 22.05.2018.

THIN GALLIUM NITRIDE FILMS ON A^{III}B^V SEMICONDUCTOR SURFACES: PREPARATION, POSSIBLE APPLICATIONS

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Owing to their chemical stability, thin surface films of GaN are promising to be used for improvement of the electronic and optoelectronic devices based on A^{III}B^V semiconductors. Such films should provide an effective protection of the crystalline semiconductor surfaces against oxidation in air or against chemical interaction with components of growth ambient in MBE chamber. However, because of the high value of the lattice mismatch (~ 20 % for GaN and GaAs) nitride films loose mechanical stability and coherency with the substrate lattice when their thickness becomes almost two monolayers. The extremely small thickness of the nitride surface films is also vital to provide electron transparency of the films and their compatibility with various device technologies. On the other side, conventional nitridation techniques using nitrogen plasma provide only formation of strongly defected and thick GaN layers.

We developed a wet chemical nitridation procedure in hydrazine–sulfide solutions which allows us to create monolayer films of GaN on GaAs and GaSb surfaces [1]. Formation of the GaN films results from selective adsorption of the nucleophilic components of the solution on the Ga- and As-related surface adsorption centers. At the beginning, adsorption of SH-anions results in removal of the surface oxide layer together with a layer of surface As atoms. Then dissociative adsorption of hydrazine molecule on the opened Ga- surface atoms results in formation of the surface GaN monolayer. Performed investigations confirm that the wet chemical nitridation procedure produces an effective surface chemical passivation of GaAs and GaSb crystals [1]. Finally, a number of possible applications of the nitride films including passivation of GaAs nanowires are demonstrated [2].

References

- [1] V. L. Berkovits, A. B. Gordeeva, T. V. L'vova, V. P. Ulin. *Semicond.*, 2012, 46, 1432.
- [2] P. A. Alekseev, M. S. Dunaevskiy, V. P. Ulin, T. V. Lvova, D. O. Filatov, A. V. Nezhdanov, A. I. Mashin, V. L. Berkovits. *Nano Lett.*, 2015, 15, 63.

CHELATE CHROME AND ZINC IN WARM CULTIVATION

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Today improvement of environmental ecological conditions and the population's health, are global problems. For resolving this problem, it is very important to produce ecologically safe agricultural products in which warms can play significant role. It's very important to study the influence of various factors on the growth of protein mass and reproduction quality for warms [1 – 3]. For this purpose the experiments were conducted, for which we synthesized (1) chelate chrome with methionine and (2) chelate zinc with methionine minimal (min), normal (norm) and maximum (max) doses in g and then the substrate of the warms was saturated with these chelates.

During the whole period of both experiments, in all groups, the weight of worms was increased. In addition, compared to the controller, all test groups have the mass increase high quality and it reaches the maximum for the chrome chelate in the 1st test group (min) 106.19 %, and for zinc chelate in the 2nd group (norm) – 107.32 %. As for the increase of reproduction quality of cocoons for both cases, compared to all the test groups are higher and reaches maximum for the chrome chelate in 3rd test group (max) – 142.59 %, but for the zinc chelate in 1st test group (min) – 152.87 %. Based on the results, obtained from the analysis, optimal and affective dose is established for chrome chelate 0.0028 g for 300 g of substrate and for zinc chelate – 0.0269 g for 300 g substrate. So, balancing the warms substrate with chelate chrome and chelate zinc makes positive influence on the warm's weight growth and greatly increases cocoons reproduction quality.

The obtained results, we think have a great importance for development of warm cultivation where the protein mass is used to balance the combined food of agricultural animals and birds as a vitamin-protein, high-quality, concentrated supplement.

References

- [1] I. N. Titov, V. M. Usoev. Bull. Tomsk State Univ., 2012, Biology Ser., 2.
- [2] C. A. Edwards, A. A. Niederer, N. Q. Arancon, R. N. Sherman. In: Vermiculture Technology: Earthworms, Organic Wastes, and Environmental Management, 2011, CRS Press – Taylor & Francis Group, 323.
- [3] I. Beshkenadze, M. Gogaladze. U1956, Geo Patent, 02.02.2016.

LOW TEMPERATURE DOPING OF GALLIUM NITRIDE NANOLAYERS

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As it is known, the third group nitrides are wide band gap semiconductors. They are primarily used as the basic material for light emitted diodes and optoelectronic devices working in the ultraviolet spectral range. In addition, their radiation resistance is also important. But it is also known that in nitride films, which are formed at high temperatures (900 – 1100 °C), is a difficult to create the p-n junction, because of difficulty to get p-type nitride. To solve this problem, it is important to research and process methods of forming and modifying nitrides. One of the main methods of modifying semiconductors is their doping by different impurities.

In the present work, there are investigated possibilities, in the process of low-temperature growing, doping gallium nitride (GaN) for obtaining p-type conductivity. As a dopant materials were selected indium (In), silicon (Si), magnesium (Mg), iron (Fe) and copper (Cu). The experiments were carried out at a low-temperature ($T \leq 700$ °C) by the original method developed by us. Studies have shown that Fe and Cu impurities allow p-type conductivity, which make them to use for receiving p-n junction and appropriate optoelectronic devices.

HEAVY HOLE- AND LIGHT HOLE-TRION STATES IN ELLIPSOIDAL QUANTUM DOT

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The negative trion, which consists of two electrons bound by a hole, is the semiconductor analogue of the hydrogen ion H^- . As the exciton is neutral, its attraction is very weak the trion can only be observed at very low temperatures. Hence, the existence of trions was proposed more than 50 years, but it was only, in the 1990's, identified in semiconductor quantum wells [1 – 4].

As is well known, the reduced dimensionality enhances considerably the binding energy of charged excitons, and thus facilitates the experimental observations. In this context the investigation of negative trions in semiconductor quantum dots (QD) is very promising. QDs are structures in which the charge carriers (electrons or holes) are confined in all three dimensions. In such nanometer QDs, some novel physical phenomena and potential electronic device applications have generated a great deal of interest [5 – 8]. We will consider heavy hole and light hole negative trions in strongly prolate ellipsoidal quantum dot (SPEQD).

The ground state of the negative trion is a singlet state; therefore, ground state spatial trial wave function of the negative trion is symmetric with respect to the interchange of the position vectors of the electrons (holes).

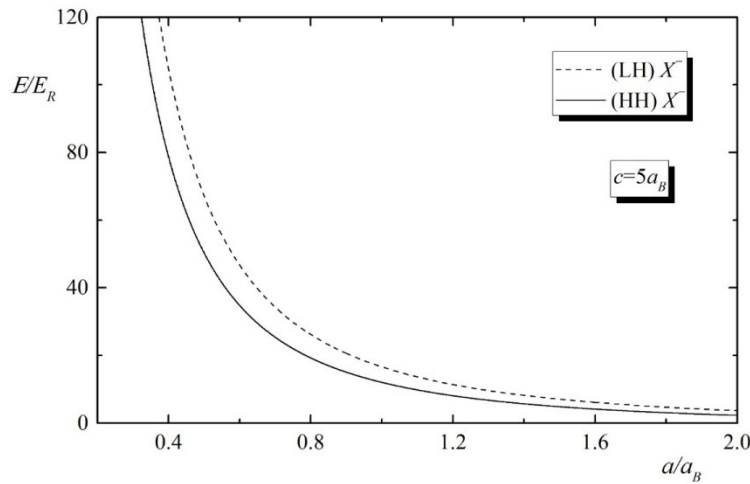


Figure 1. Dependencies of heavy hole and light hole negative trions on small semiaxis.

The variation function for the negative trion will be constructed on the single-particle wave functions and will have the following form [9]:

$$\Psi_{trial}(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_a) = C \psi_{100}(\vec{\rho}_1) \psi_{100}(\vec{\rho}_2) \psi_{100}(\vec{\rho}_a) \times \sum_{i_1 i_2} \sum_{j_1 j_2} c_{i_1 i_2 j_1 j_2} (1 + P_{12}) e^{-\alpha_1^{1a} \rho_{1a}^2 - \alpha_2^{1a} \rho_{2a}^2 - \alpha_{12}^{12} \rho_{12}^2} \times e^{-\beta_1^{1a} z_{1a}^2 - \beta_2^{1a} z_{2a}^2 - \beta_{12}^{12} z_{12}^2}, \quad (1)$$

where C is normalization constant, $\rho_{jk} = |\vec{\rho}_j - \vec{\rho}_k|$, $j, k = \{1, 2, a, b\}$, α , β , and γ are variational parameters. These parameters can be determined after minimizing the integral:

$$E_{X^-} = \langle \Psi_{trial}(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_a) | \hat{H} | \Psi_{trial}(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_a) \rangle. \quad (2)$$

Here \hat{H} is the Hamiltonian of the system, which is described by the following form:

$$X^-, \hat{H} = \sum_j \frac{\hat{P}_j^2}{2m_j^*} + V_{int}(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_a) + \sum_j U_{conf}(\vec{\rho}_j, z_j), \quad j = \{1, 2, a\}. \quad (3)$$

By the help of the variation method one can calculate the energy of negative trions for the ground level (**Figure 1**).

Let us proceed to the calculation of the binding energy. For two types of negative trions, expressions for the binding energy are defined below:

$$\begin{aligned} E_{bind}(X_\ell^-) &= (2E_e + E_{\ell h}) - E(X_\ell^-), \\ E_{bind}(X_h^-) &= (2E_e + E_{hh}) - E(X_h^-). \end{aligned} \quad (4)$$

where E_e , $E_{\ell h}$ and E_{hh} are the energies of the electron, light hole and heavy hole respectively, in the SPEQD.

As the next step let us calculate the recombination energies of negative trions, calculated according to the following formulas:

$$\begin{aligned} \omega_{if}(X_\ell^-) &= E^{(i)}(X_\ell^-) - E_e^{(f)}, \\ \omega_{if}(X_h^-) &= E^{(i)}(X_h^-) - E_e^{(f)}, \end{aligned} \quad (5)$$

where indices i and f are the initial and final states, respectively. The recombination energy is defined as a difference between the total energies of the initial and final states after recombination.

References

- [1] W. Xie. Chem. Phys., 2012, 408, 69-74.
- [2] M. A. Lampert. Phys. Rev. Lett., 1958, 1, 450.
- [3] B. Stebe, A. Ainane. Superlatt. & Microstruc., 1989, 5, 545.
- [4] A. J. Shields, M. Pepper, M. Y. Simmons, D. A. Ritchie. Phys. Rev. B, 1995, 52, 7841.
- [5] B. Stebe, A. Ainane, F. Dujardin. J. Phys. Cond. Matter, 1996, 8, 5383.
- [6] W. Xie. Solid State Comm., 2001, 118, 305.
- [7] E. Anisimovas, F. M. Peeters. Phys. Rev. B, 2003, 68, 115310.
- [8] C. Riva, F. M. Peeters, K. Varga. Phys. Rev. B, 2000, 61, 873.
- [9] B. Szafran, B. Stebe, J. Adamowski, S. Bednarek. Phys. Rev. B. 2002. 66, 165331.

ABSORPTION AND FLUORESCENCE SPECTROMETRY FOR ANALYSIS OF QUALITY OF DNA DOUBLE HELIX

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The aim of this work is to demonstrate the significance of the phenomena of light re-radiation and the electron excitation energy transfer from the donor to the acceptor in the hydrolysis reactions of glycoside and phosphodiester bonds in DNA, which is important for the functionality of cells in the norm and pathology and for the analysis of the quality of the double helix DNA for diagnostic purposes.

It is shown that photons of the near-IR region of the spectrum excite the overtones of the large-amplitude valence vibration of water molecules in the 700 – 1500 nm spectral range. This causes the activation of electrolytic dissociation of water molecules with the formation of H⁺ and OH⁻, which is necessary for the hydrolysis reaction of chemical bonds in biological molecules.

The application of the original nanoscale method of a laser induced fluorescence resonance energy transfer to a donor-acceptor intercalator pair for the quantitative and qualitative study of stability quality DNA double helix in a solution, in real time is shown in the following biologically important processes: photo-irradiation, photodynamic effect and electron excitation energy transfer in strongly scattering environment (colloidal) with multiple scattering of light, i.e. in processes that can be successfully used in light therapy of cancer, dermatology, wound healing, etc.

NEW BILAYER GRAPHENE-LIKE NANOSTRUCTURES WITH NANOHOLES: MODELLING, EXPERIMENTS, AND APPLICATIONS

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Recently, graphene and other quasi-two-dimensional materials (hexagonal boron nitride-h-BN, phosphorus, silicene and transition metal dichalcogenides) [1, 2] together with van der Waals heterostructures (several such layers in combination with graphene) attract great interest because of the prospects of their applications in nanoelectronics and optoelectronics. They have remarkable properties that may not occur in their individual constituent layers.

In this review, it is proposed to highlight some of the latest developments in the electronic, mechanical and optoelectronic properties of graphene-based heterostructures: two-layer graphene (BG) and graphene / h-BN structures, as well as their analogs with “closed” holes [3 – 6], features of their semimetallic, metallic and semiconductor properties.

Different stable forms of nanoholes with closed edges are studied in BG layered and nanoribbon structures of AA, AB and Moiré stacking with closed edge holes: atomic structures and electronic properties. The most advantageous shape of the BLG holes was determined in a manner analogous to the method used by G. Wulff to find the optimal shape of the crystals, which can also be used to determine the shape of the pores for two-dimensional crystals. The comparisons of modeling examples with experiments are made [3, 5, 7, 8]. Nanostructured few-layer graphene films with interlayer edge reconstruction (by high-energy Xe⁺ ions) for electronic applications were considered by experimentally and theoretically [6]. The graphene / h-BN structures with nanoholes and their unique properties are also considered [4].

Prospects and possible applications of such materials in nanoelectronics and electro-optics, mechanical, biomedical, and photovoltaic devices are discussed.

References

- [1] K. S. Novoselov, et al. Science, 2016, 353, 6298.
- [2] L. A. Chernozatonskii, A. A. Artyukh. Physics – Uspekhi, 2018, 61, 2.

- [3] L. A. Chernozatonskii, V. A. Demin, Ph. Lambin. Phys. Chem. & Chem. Phys., 2016, 18, 27432.
- [4] L. A. Chernozatonskii, V. A. Demin, S. Bellucci. Sci. Rep., 2016, 6, 38029.
- [5] L. A. Chernozatonskii, A. A. Artyukh, Phys. Rev. B, 2018 – *in preparation*.
- [6] N. A. Nebogatikova, I. V. Antonova, S. V. Erohin, D. G. Kvashnin, A. Olejniczak, V. A. Volodin, A. V. Skuratov, A. V. Krasheninnikov, P. B. Sorokin, L. A. Chernozatonskii. Nanoscale, 2018, 10, 14499.
- [7] E. Moyen, A. Hama, E. Ismailova, L. Assaud, G. Malliaras, M. Hanbucken, R. M. Owens. Nanotechnol., 2017, 27, 074001.
- [8] Ph. S. Mahapatra, K. Sarkar, H. R. Krishnamurthy, S. Mukerjee, A. Ghosh. Nano Lett., 2017, 17, 6822.

SYNTHESIS OF AMINO ACID BASED UNSATURATED BIODEGRADABLE POLY(ESTER AMIDE)S WITH DOUBLE BOND MOIETIES IN BACKBONES

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The α -amino acid based (AAB) poly(ester amide)s (PEAs) belong to the class of AA–BB type heterochain polymers obtained by solution active polycondensation [1 – 3]. Besides the diversity in material properties, they have shown good biocompatibility and low inflammatory response [4], which makes PEAs highly attractive for biomedical applications.

One of the most convenient ways to functional polymers is the incorporation into the polymeric backbone unsaturated double bonds that could easily be derived [5]. Unsaturated PEAs (UPEAs) were synthesized using in solution active polycondensation di-*p*-nitrophenyl fumarate as a bis-electrophilic partner of di-*p*-toluenesulfonic acid salts of bis-(α -amino acid)- α,ω -alkylene diesters – key monomers for preparing AAB–PEAs [6].

The syntheses of three types of new unsaturated PEA polymers were explored – (i) Leu- and Phe-based unsaturated PEA homopolymers (UPEAs) composed of 100 % of fumaric acid, (ii) Leu-based unsaturated-saturated copolymers (USPEAs) composed of fumaric acid and saturated fatty diacids, and (iii) Leu- and Phe-based UPEA copolymers composed of 100 % fumaric acid (co-UPEAs).

The UPEAs were further chemically modified into functional derivatives as well as subjected to thermal and photochemical transformations (curing) that substantially expand material properties and, hence, the scopes of potential applications of α -amino acid based biodegradable poly(ester amide)s as absorbable surgical devices and drug carriers.

References

- [1] R. Katsarava, V. Beridze, N. Arabuli, D. Kharadze, C. C. Chu, C. Y. Won. J. Polym. Sci. A, 1999, 37, 391–407.
- [2] Z. Gomurashvili, R. Katsarava, H. R. Kricheldorf. J. Macromol. Sci. A, 2000, 37, 215–227.
- [3] M. Okada, M. Yamada, M. Yokoe, K. Aoi. J. Appl. Polym. Sci., 2001, 81, 2721–2734.
- [4] S. H. Lee, I. Szinai, K. Carpenter, R. Katsarava, G. Jokhadze, C. C. Chu, Y. Huang, E. Verbeken, O. Bramwell, I. De Scheerder, M. K. Hong. Coronary Artery Disease, 2002, 13, 237–241.
- [5] X. Lou, C. Detrembleur, P. Lecomte, R. Jerome. e-Polymers, 2002, No 034.
- [6] E. Chkhaidze, D. Tugushi, D. Kharadze, Z. Gomurashvili, C. C. Chu, R. Katsarava. J. Macromol. Sci. A, 2011, 48, 544–555.

SEMICLASSICAL MODEL OF MULTIELECTRON ATOMS: ELECTRONIC STRUCTURE CALCULATIONS

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There is suggested a new semiclassical model for multielectron atoms describing the atomic electron-states in terms of hydrogen-like orbitals.

Based on the constituent atoms semiclassical electron-orbitals, the electronic structure of molecules, nanosystems, and condensed matter can be calculated analytically expressing the quantum-chemical integrals by special functions.

GOLD NANOPARTICLE AND FLUORESCENT DYE DECORATED CALMODULIN AND PROSTATE SPECIFIC MEMBRANE ANTIGEN PROTEINS AS CONTRAST AGENTS IN BIOLOGICAL TISSUES

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Functionalized gold nanoparticles with controlled optical properties are the subject of intensive studies and biomedical applications, including genomics, biosensors, immunoassays, clinical chemistry and laser phototherapy of cancer cells, the targeted delivery of drugs, optical bioimaging and the monitoring of cells [1].

In this work, we propose two nanocomposites consisting of gold nanoparticle (GNP) and fluorescent dye decorated proteins, which can serve as the contrast agents for the detection of diseases at the early stage of development, using the simple and inexpensive imaging methods. As the proteins targeted by GNPs and fluorescent dyes, we selected Calmodulin (CaM) and Prostate specific membrane antigen (PSMA).

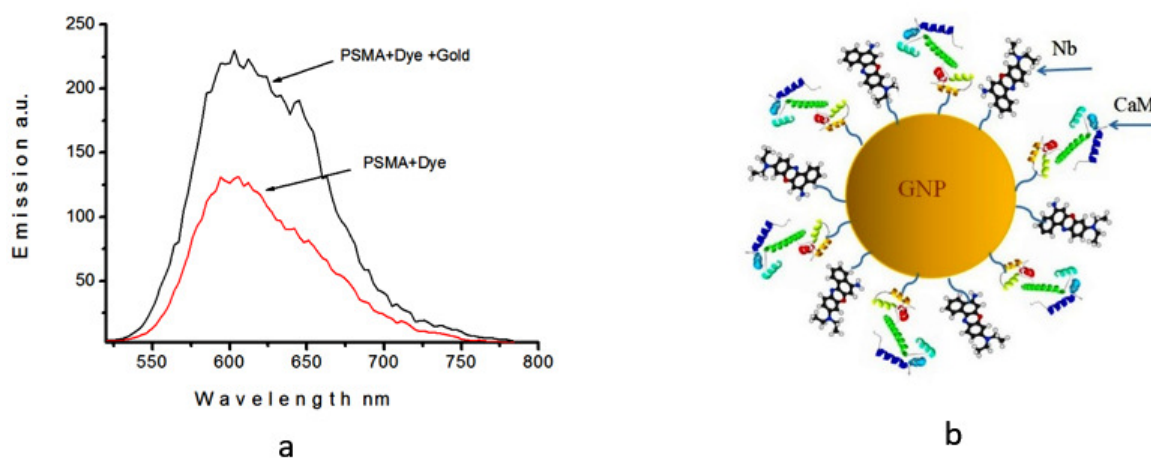


Figure 1. Light emission enhancement in GNP/PSMA/dye nanocomposite (a) and schematic illustration of GNPs functionalized with the fluorescent dye and CaM (b).

During the experiments, we have prepared and investigated CaM, PSMA and GNPs based nanocomposites and demonstrated that CaM and PSMA conjugated with fluorescent dye and GNPs can increase the fluorescence intensity upon the excitation of pumping laser source. (**Figure 1**).

Besides, we have shown that the fluorescence enhancement strongly depends on (1) size, shape, and concentration of GNPs; (2) distances between GNRs, fluorescent dyes and CaM/PSMA; and (3) relative spectral positions between the plasmon absorptions of GNPs and the absorption and emission of the fluorescent dyes [2]. This ability of controlled targeting and visualization of CaM/PSMA by fluorescence can be beneficially used in the tracking of CaM and PSMA mediates processes in biological tissues and cells, such as inflammation, metabolism, apoptosis, muscle contraction, intracellular movement, malignant cells growth, etc.

References

- [1] L. A. Dykman, N. G. Khlebtsov. Gold nanoparticles in biology and medicine: recent advances and prospects. *Acta Nature*, 2011, 3, 2(9), 34-55.
- [2] K. Chubinidze, B. Partsvania, T. Sulaberidze, A. Khuskivadze, E. Davitashvili, N. Koshoridze. Luminescence enhancement in nanocomposite consisting of polyvinyl alcohol incorporated gold nanoparticles and Nile blue 690 perchlorate. *Appl. Opt.*, 2014 53, 31, 7177-7181.

NUMERICAL CALCULATIONS OF IMPURITY SCATTERING MOBILITY IN SEMICONDUCTORS

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Novel semiconductor-base nanotechnology is gradually moving into new applications in the world economy. Semiconductor application requires increasing of investigations in the direction of their properties. The main criterion of semiconductor suitability for application in semiconductor devices electrical properties, particularly current carriers' mobility. Therefore, the problem connected with the explanation of the experimental results of charge carriers' mobility on the base of theoretical complicated formulas is very urgent.

In the current paper, current carriers' mobility due to ionized impurity scattering is discussed and calculated using numerical methods. Calculations were done for different temperatures and different range of current carriers concentration.

NANOTECHNOLOGICAL APPROACH FOR MONITORING OF GM MAIZE

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The development of efficient methods for the monitoring of genetically modified organisms (GMOs) is of crucial importance for the environment and human health protection, food labeling and safety assessment. Genetically modified (GM) maize is among major GM crops. In this study a new nanotechnological approach namely multiplex polymerase chain reaction (PCR) coupled with low-density DNA microarray (biochip) was developed for fast, cheap and reliable identification of GM maize varieties such as Bt-176 and MON 810.

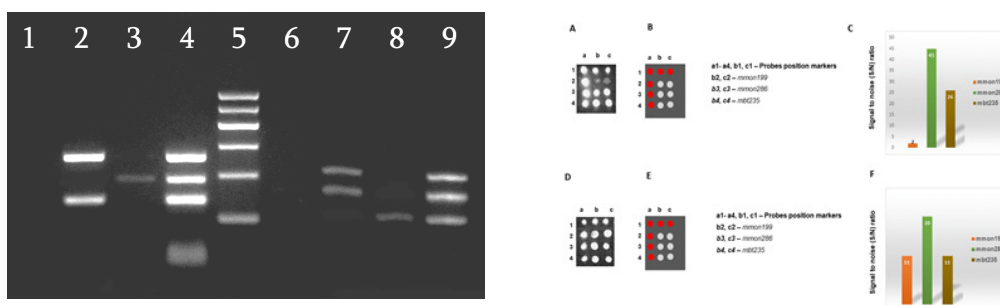


Figure 1. Agarose gel for multiplex PCRs. **Figure 2.** Microarray image analysis.

New PCR primers and suitable DNA probes were designed using bioinformatics tools. The products of multiplex PCRs were analyzed by agarose gel electrophoresis (**Figure 1**). The sensitive 3D platform dendrimeric matrixes with new DNA probes were manufactured and used in hybridization with multiplex PCR amplicons (**Figure 2**). Multiplex PCR results and microarray image analysis demonstrated that new biochips and multiplex PCR methods allow simultaneous detection of the junction region between maize genome and GMO-specific cauliflower mosaic virus (CaMV) 35S promoter in MON810, the junction region between transgenic Cry1Ab delta-endotoxin (cry1Ab) gene and maize genome in MON810 and the junction region between transgenic bar gene and maize genome in Bt-176. Analysis of foodstuffs indicated that new nanotechnological approach developed in this study may be used for reliable and fast tracing of GM maize events MON 810 and Bt-176 in foods.

ANALYSIS OF VORTEX DYNAMICS OF ELECTROLYTE IN DC MAGNETIC FIELD

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In recent years, a growing interest in the field of electrochemistry is related to the study of processes occurring at the ferromagnetic-electrolyte interfaces, in particular, the phase separation of electrolyte in an external magnetic field. Such processes depend on both the gradient of magnetic field and its distribution on the metal surface.

Earlier [1, 2] the optical investigations of formation of the dispersed phase in electrolyte and the dynamic characteristics of its motion both in infrared and visible irradiation were carried out. The performed study allowed obtaining the distributions of the characteristic frequencies of the electrolyte motion over the volume of the medium under investigation.

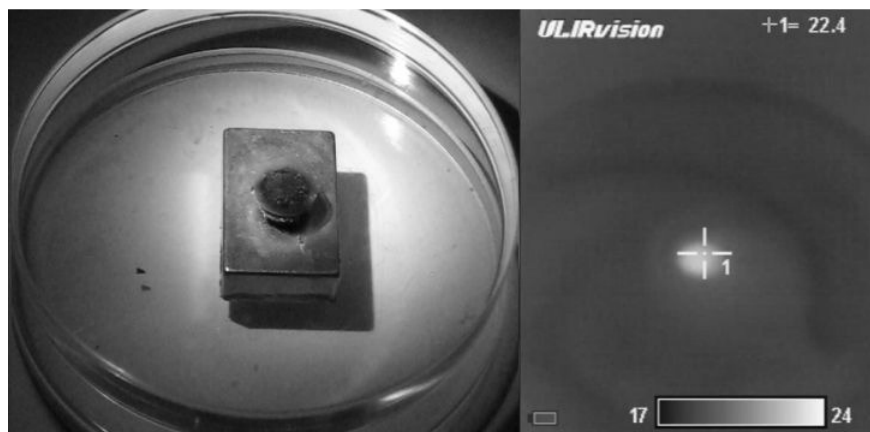


Figure 1. Thermal imager ULIR-vision TI-384.

In the present study, the motion of the electrolyte under different configuration of the magnetic field was investigated, and the distribution of the temperature gradients arising during the reaction was studied using the thermal imager ULIR-vision TI-384 (**Figure 1**).

References

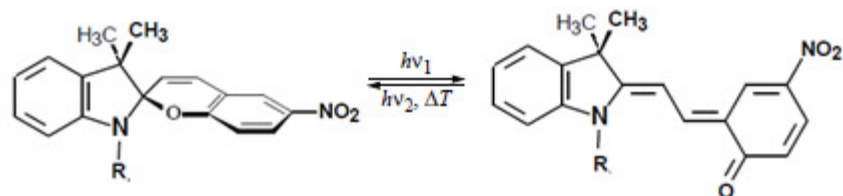
- [1] D. O. Derecha, Yu. B. Skirta, I. V. Gerasimchuk. J. Phys. Chem. B, 2014, 118, 50, 14648.
- [2] D. O. Derecha, Yu. B. Skirta, I. V. Gerasimchuk. Nanoscale Res. Lett., 2015, 10, 440.

HIGHLY PHOTSENSITIVE AND RADIANT ENERGY-SAVING MOLECULAR SWITCHES

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The work proposes highly photosensitive and stable molecular switches created through the integration by the improved method of microcapsulating designed by us [1] in the polymer of nemato-chiral liquid-crystal compositions doped with bistable, so called long-radical spiropyrans (II), which help economize the electrical power needed for the photoinduction occurring during the photochromic transformations.



R = CH₃ (I) and R = C₁₄H₂₉ (II)

The work is based on an event of nanostructuring of merocyanine molecules into the spherical micelles, which are formed as a result of photoinduction with the ultraviolet (UV) light. Nanostructuring increases the effective photosensitivity of the composition [2].

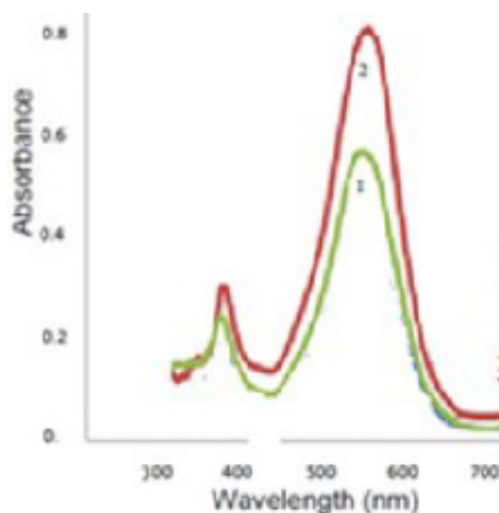


Figure 1. Absorption spectra of UV photoinduced spiropyrans I (1) and II (2).

The pseudo-phase formed in the solution at a nano-level by the UV photoinduction, the micelles, deplete the base solution off merocyanine molecules and as a result, spiropyran

molecules start to transform into the merocyanine molecules to restore the thermodynamic equilibrium. The merocyanine molecules formed photochemically are added by the molecules formed to restore the thermodynamic equilibrium i.e., from this moment, the process takes place at the expense of the internal energy and the coloration of the system continues without the consumption of the radial energy (**Figure 1**).



Figure 2. Polymer films doped compounds I **(a)** and II **(b)**.

This result was clearly seen, when recording the image on the polymer films (see the **Figure 2**).

References

- [1] K. Japaridze, Ts. Zurabishvili, G. Petriashvili. Georgian Patent P 5232, 2011.
- [2] K. Japaridze, L. Devadze, J. Maisuradze, G. Petriashvili, Ts. Zurabishvili, I. Mzhavanadze, N. Sepashvili. Bull. Georg. Natl. Acad. Sci., 2013, 7, 3, 57-62.

MULTI-COMPONENT REACTION, SOLVENT-FREE SYNTHESIS OF SUBSTITUTED PYRANO-PYRIDO PYRIMIDINE UNDER DIFFERENT CONDITIONS USING ZnO NANOPARTICLES

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The 2-amino-4-(4-substitutedphenyl)-5-oxo-4H,5H-pyrano [2,3-d] pyrido [1,2-a] pyrimidine-3-carbonitrile derivatives 2-12 [**1** – **3**] were synthesized via multi-component condensation reaction of different aromatic aldehydes (**Figure 1**), 3H-pyrido[1,2-a]pyrimidine-2,4-dione 1 and malononitrile by using ZnO nanoparticle as green, environmentally friend catalyst under solvent-free conditions.

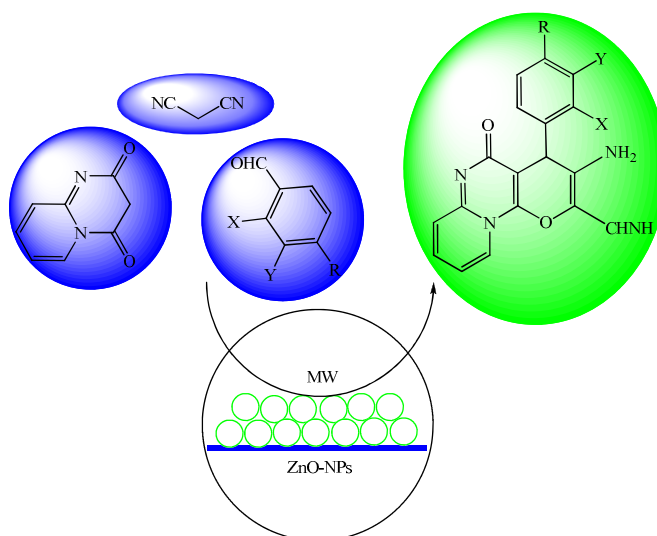


Figure 1. Multi-component condensation reaction of aromatic aldehydes.

The present work creates a variety of biologically active heterocyclic compounds in excellent yield and short times. The structures of all compounds were elucidated with the elemental analysis, IR, ¹H-NMR, and mass spectral data.

References

- [1] M. Ghashang, M. Kargar, M. R. M. Shafiee, S. S. Mansoor, A. Fazlinia, H. Esfandiari. Recent Pat. Nanotech., 2015, 9, 204-211.
- [2] M. Ghashang. Lett. Org. Chem., 2012, 9, 497-502.
- [3] N. Maleki, Z. Shakarami, S. Jamshidian, M. Nazari. Acta Chem. IASI, 2016, 24, 1, 20-28.

NATURAL NANOMATERIALS – MELIORANTES OF OIL-POLLUTED SOILS

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When solving the problem of re-cultivation of oil polluted soils, it seems more expedient to develop methods for stimulating the activity of native oil-assimilating microflora of polluted soil. These methods do not require laborious, costly operations associated with releasing, cultivation and introduction of a hydrocarbon-oxidizing microorganism culture [1]. The greatest effect in this case can be achieved through the use of environmentally safety meliorants, for example, natural zeolites which simultaneously provide the sorption of petroleum hydrocarbons and the adhesion of cells of oil-assimilating microorganisms from soil.

In this paper, the effect of natural zeolite (clinoptilolite) introduced into oil-polluted soil on the growth and development of a test plant was studied. Zeolite is a macromolecular system with a developed surface, the activity of which is due to the molecular-sieve effect of micropores [2].

The experiment was carried out on grey-brown soil. The soil was polluted with oil from the Samgori field (Georgia). The degree of soil contamination with oil was 2.5; 5.0 and 10 % of the mass of the soil natural zeolite-clinoptilolite containing tuff of the Tedzami origin, the Handaki section of Georgia, with a main mineral content of 70 – 80 %. Eight types of the experiments were performed, each in four repetitions. In laboratory conditions, experiments were conducted to study the effect of oil products and zeolites on laboratory germination, germination energy, and the formation of the vegetative mass of the test culture. Experimental data showed that the application of zeolite has a meliorative effect on the soil and improves the biometric parameters of the test culture in comparison with the indices of the culture grown on contaminated soil. The energy of germination of the test culture on the substrate rises an average of 10 – 40 % and germination capacity by 60 %. Energy of germination of test culture was determined on the fourth day, and the germination capacity on the tenth day after sowing.

References

- [1] Eds. N. A. Anjum, M. E. Pereira, I. Ahmad, A. C. Duarte, Sh. Umar. In: Nafees Phytotechnologies: Remediation of Environmental Contaminants, 1998, 109.
- [2] L. Eprikashvili, T. Kordzakhia, M. Dzagania, M. Zautashvili, N. Pirtskhalava. The restoration of soil ecosystems by natural zeolites. Nano Studies, 2016, 14, 77-84.

NANOMODIFIED ZEOLITE IN COMPOSITION OF COMPLEX FERTILIZER

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Nowadays, nanomaterials and nanotechnologies are used practically in all fields of agriculture: crop production, animal husbandry, poultry farming etc. The use of nano-products in crop production as micro-fertilizers provides an increase of productivity (on average 1.5-2 times) for almost all food cultures [1]. Zeolites are nanoporous crystalline solids and have a frame structure with an alumino silica-oxygen basic motif [2]. The aim of the research was the possibility to improve the agrochemical and biological characteristics of the soil under the influence of organic-mineral fertilizer: modified (NH_4^+ and K^+) zeolite + lignite (source of humid substances [3]) and its influence on some biometric test cultures. The following biometric indicators were determined: the germination energy (GE), the relative value of the germination energy (RVGE), germination capacity (GC), the relative value of germination capacity (RVGC) of seeds. The greatest increase in GE and GC occurs when zeolites, modified with potassium and ammonium cations and brown coal are used during the third sowing. Enrichment of the soil with substrates affects the growth of both the above-ground part and the root system of the plant, although this difference on different substrates occurs differently. The root system develops more on the substrate: soil + zeolite and brown coal + zeolite, and the aboveground part on the substrate – soil + modified zeolite. A large difference is also observed in case of brown coal + modified zeolite. Differences were also noticed in the dry mass of plant, both the aboveground part and the root system, which demonstrate an increase in the growth of plants grown on the studied substrates. Further investigation in this direction is very actual from an ecological point of view. It contributes to the utilization of substandard coal industry wastes as organic components for increasing soil fertility.

References

- [1] Comp. N. I. Kugutina. Nanotechnologies in Agriculture (Prospect), 2012, Kursk, N. N. Aseev Kursk Reg. Sci. Library, 19 pp.
- [2] V. C. Radkovski, E .C. Actapova, A. V. Filimonov. Formations of physical and chemical properties of zeolite-nanoparticle system during mechanical activation. Sci. & Tech. Bull. (Phys. & Math. Sci.), 2011, 4, 16-24.
- [3] P. J. Leggo. The organo-zeolitic-soil system: A comprehensive fertilizer. Int. J. Waste Resources, 2014, 4, 3.

SYNTHESIS AND PROPERTIES OF $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ NANOPARTICLES BY SONOCHEMICAL METHOD

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The synthesis and characterization of II–VI group semiconductor compounds have attracted considerable attention in recent years due to wide applications and variable bandgap energy. The $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ ternary compound has significantly application such as solar cells, photodetectors, lasers and other opto-electronic devices [1]. Synthesis of $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanoparticles with varying samples concentrations ($x = 0, 0.2, 0.4, 0.5, 0.6, 0.8$, and 1) allow that the optical bandgap of $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ to change between band gap values of ZnS and CdS [2]. In this paper we studied optical, structural properties and morphology of $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanoparticles.

The $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanoparticles were synthesized by sonochemical method in aqueous medium at air conditions. Appropriate amount of $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$, $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ as cation source, $\text{Na}_2\text{S} \cdot 9\text{H}_2\text{O}$ as anion source and polyvinyl alcohol (PVA) as capping agent were used. The Cd^{2+} and Zn^{2+} molar ratios were as 1:4 and 2:3. Capping agent was prepared 2 % water solution. All reagents were dissolved in distilled water. The reaction was carried out in air atmosphere for 2 h. The final sample color was light yellow. The sample resulting of reaction was separated by centrifugation and washed three times with distilled water and dried at room temperature.

The synthesized $\text{Cd}_{0.2}\text{Zn}_{0.8}\text{S}$ and $\text{Cd}_{0.4}\text{Zn}_{0.6}\text{S}$ nanoparticles were obtained in cubic crystal structure by X-ray diffractometer (XRD). The nanoparticles sizes were defined by Debye Scherrer equation from XRD results and scanning electron microscopy (SEM) images. The particle sizes of $\text{Cd}_{0.2}\text{Zn}_{0.8}\text{S}$ and $\text{Cd}_{0.4}\text{Zn}_{0.6}\text{S}$ were calculated 1.78 and 2.14 nm, respectively, by XRD and for $\text{Cd}_{0.4}\text{Zn}_{0.6}\text{S}$ nanoparticles was 10.4 – 15.8 nm by SEM images. The values of the optical band gap energies of $\text{Cd}_{0.2}\text{Zn}_{0.8}\text{S}$ and $\text{Cd}_{0.4}\text{Zn}_{0.6}\text{S}$ nanoparticles were found to be 2.80 and 2.45 eV, respectively. It was clear that from energy dispersive X-ray spectroscopy (EDX) the ratio of ions which entered into the solution was same compilation in nanoparticles. The results show that initial reagents were spent totally formation of the sample. As seen from results the optical band gap values decrease with increase of particles size.

References

- [1] P. Kumar, A. Misra, D. Kumar, N. Dhama, T. P. Harma, P. N. Dixit. Opt. Mater. 2004, 27, 261-264.
- [2] T. L. Chu, S. S. Chu, J. Britt, C. Ferrikide, O. Q. Wu. J. Appl. Phys., 1991, 70, 2688-2693.

SUPERCONDUCTING GAP IN Ca122 IRON-BASED SUPERCONDUCTORS REVEALED BY POINT-CONTACT ANDREEV REFLECTION SPECTROSCOPY

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We present the point-contact Andreev reflection study of the iron-based single crystals $\text{Ca}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ (Ca122) with $x = 0.04$ and 0.10 , which become superconducting below $15 - 17$ and 20 K respectively. The point contacts based on the above-mentioned samples were formed by touching a clean thin sharpened Cu wire to the cleaved surface of the bulk sample [1]. The resistance of such point contacts was in the range from several Ohms to tens of Ohms that corresponded to the contacts' size from several to hundreds of nanometers, thus, forming a nanoobject between two bulk materials. The measurements of current-voltage ($I - V$) characteristics of the point contacts and their first derivatives (dV/dI) were carried out in the temperature range $3 - 20$ K using the standard lock-in technique [1].

We selected dV/dI spectra, which demonstrate the Andreev-like double minima structure below the superconducting critical temperature. The minima located in the energy range between 5 and 10 meV transform to a single minimum with temperature increasing, and disappear above the critical temperature. Normal state of dV/dI shows usually a zero-bias maximum of Kondo type, probably due to scattering on non-stoichiometric Fe or Co magnetic impurities. The fit of dV/dI spectra within BTK model [2] results in the one gap with $2\Delta/k_B T_c \approx 5$ and 10 for the samples with $x = 0.04$ and 0.10 , respectively. Comparing our results with the literature data one can see a large variation of the reduced gap values: from $2\Delta/k_B T_c = 2 - 4$ and $5 - 10$ for two gaps in Ba122 and Ca122 [3 – 6] up to $2\Delta/k_B T_c \sim 15$ for Ca122 in [7]. Moreover, the broad distribution of the both gaps within a nanometer scale connected with impurity scattering in $s\pm$ -superconductors [8]. Thus, our data are in the line with this scenario, while non-ideal interface at point-contact formation enhances impurity scattering, which is seen by observation of the mentioned above Kondo maximum.

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References

- [1] Y. G. Naidyuk, I. K. Yanson. Springer Series in Solid-State Sciences, 145: Point-Contact Spectroscopy, 2005, New York: Springer.
- [2] G. E. Blonder, M. Tinkham, T. M. Klapwijk. Phys. Rev. B, 1982, 25, 4515.
- [3] P. Samuely, et al. Physica C, 2009, 469, 507.
- [4] M. Tortello, et al. Phys. Rev. Lett., 2010, 105, 237002.
- [5] R. S. Gonnelli, et al. Supercond. Sci. & Technol., 25, 2012, 065007.
- [6] D. Daghero, et al. Low Temp. Phys., 2013, 39, 261.
- [7] P. Kumar, et al. J. Phys. Cond. Matter, 2011, 23, 255403.
- [8] M. L. Teague, et al. Phys. Rev. Lett., 2011, 106, 087004.

STUDY OF TOXICITY OF BIOLOGICALLY SYNTHESIZED CdS QUANTUM DOTS ON HUMAN CELLS

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Quantum dots (QDs) are typical II–VI semiconductor materials, owing to their unique optical properties and tunable photoluminescence, have received much interest in the field of electronic and biomedical applications. However, the cytotoxicity of QDs has become a major concern for their safe use in bioimaging, delivery or tracking biomolecules. The role of surface chemistry of QDs is the determining factor of toxicity since surface functionalization is required for nanoparticles synthesized by conventional physical or chemical methods. But we have previously developed a novel alternative approach for the production of CdS QDs in an extra-cellular way by the biological synthesis using bacteria *Escherichia coli*, fungi *Pleurotus ostreatus* and plant *Linaria maroccana* as biomatrices. Produced nanoparticles are stable and luminescent, have a range of sizes from 2 to 10 nm in diameter. Although an important question remains to study their toxic properties in comparison with inorganic cadmium sulfide salt, because of their heavy metal composition that could cause harmful effects to human health and environment. In the present research we have evaluated cytotoxic / cytostatic effects, proliferative activity, adhesive potential of produced CdS nanoparticles using HeLa cells, tumor cells of human T- and B-lymphocytes, AGS cancer cell line by MTT-assay and flow cytometry methods. It has been found that QDs have reduced toxicity as compared to inorganic cadmium sulfide which makes them attractive as a new type of non-toxic luminescent probes for bioimaging applications in cytological studies.

STRUCTURAL STUDIES OF POLYIMIDE FILMS: SIZE EFFECT

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In connection with the rapid development of a number of areas of modern technology in recent years has sharply increased interest in the properties of polymer materials at low temperatures. The study of polymers at low temperatures is also of great importance for understanding a number of important problems in the physics of polymers [1].

The work is devoted to the study of the change in the structure of polyimide films by X-ray diffraction analysis. Structural studies were carried out on a DRON-2.0 diffractometer with Bragg-Brentano focusing in Cu K_α radiation. The plane of the sample was perpendicular to the primary of X-rays beam. The scattering intensity curves were plotted in the angular interval $2\theta = 4 - 70^\circ$ at room temperature.

The sample for the experiments was a polyimide film with a thickness of 75 and 125 μm . The samples were subjected to deformation prior to rupture at $T = 293$ and 77 K. The deformation was carried out under conditions of uniaxial tension before breaking at a deformation rate $V_{\text{def}} = 0.85 \text{ mm / min}$.

Common to the diffraction patterns obtained is the presence of reflections at small angles ($2\theta < 30^\circ$) and absence at large angles. This kind of intensity distribution indicates the presence of short-range order and the absence of long-range order in the investigated objects. However, the form of the diffraction patterns for the two thicknesses under study differs significantly. The appearance of an asymmetric peak at $\delta = 75 \mu\text{m}$ and three broad maxima at $\delta = 125 \mu\text{m}$ reflects the influence of the scale factor on the structure of the polyimide film.

The deformation of the samples at 77 K has a different effect on the distribution of the scattering intensity for samples with different thicknesses. In the case of a smaller thickness, the peaks shift toward smaller angles. In the case of a larger thickness, additional peaks appear. The authors assume that formation of regions with a lower density (compression regions) occurs in a thinner film [2]. In a thicker film, the degree of ordering of the regions increases.

References

- [1] I. I. Perepechko. Properties of Polymers at Low Temperatures, 1977, Moscow, Chemistry.
- [2] V. G. Geidarov, I. S. Braude, N. N. Galtsov, Yu. M. Pogribnaya. Effect of deformation on the structure of polyimide PM-A at low temperatures. Low Temp. Phys., 2017, 43, 10, 1537-1541.

LOCALIZED STATES IN LINEAR / NONLINEAR MEDIA OF VARIABLE PHYSICAL ORIGIN WITH TWO POTENTIAL WELLS

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As it is well known, the nonlinearity of the medium can give rise to new physical effects such as dependence of the transparency of the medium on the power of the wave being transmitted, spatial localization of nonlinear waves in periodic arrays of optical waveguides, etc. From the technological applications point of view, of special interest are layered and modulated structures of different types. In nonlinear optics, for example, where layered and modulated structures can be applied in optical communication systems, optical fibers, photonic crystals, optical delay lines, the investigations of localized states in the system with two linear / nonlinear defect layers (for instance, in optical switches) and in periodic modulated structures [1] are very actual.

The study of the adsorption of polymer chains in the system with the interfaces modeled by δ -functions or potential wells (in some cases – by nonlinear or / and asymmetric ones) is also of importance. The investigation of the structures of such type is also important in the theory of Bose–Einstein condensation.

In the present study, within the framework of nonlinear Schrodinger equation we analytically studied the nonlinear localized states in the system with two potential wells in the cases of linear and nonlinear media in the wells, as well as their linear and nonlinear environment. All possible solutions in such a system are found and studied at the conditions of continuity of the wave function and its first derivative at the boundaries of the potential wells and the environment. The exact solutions are found, and the character of localization of nonlinear stationary waves are studied for all possible combinations: (1) continuous linear medium in the system; (2) nonlinear medium in the potential wells and linear medium in the surrounding areas; (3) medium with linear properties in the potential wells and nonlinear medium in the surrounding areas; (4) continuous nonlinear medium in the system. The frequency dependences of the field amplitudes for all types of possible stationary localized states are obtained.

Reference

- [1] I. V. Gerasimchuk, A. S. Kovalev. JETP Lett., 2007, 85, 10, 488-492.

LOCALIZED NONLINEAR WAVES IN NONLINEAR MEDIA WITH INTERFACES

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The investigations of the structure and dynamic properties of multilayered systems with thin layers are of great interest now. The simultaneous influence of the layered structure of the medium and the nonlinearity give rise to new physical effects such as spatial localization of nonlinear waves in modulated structures (see, for example, [1, 2]), dependence of the transparency of a medium on the power of the wave, etc. Of special interest are layered structures of different types promising for technological applications.

We study analytically the localized states of nonlinear waves propagating along two coupled identical parallel plane defect layers (interfaces) in a nonlinear medium. In this case the nonlinear states are localized near interfaces but the densities of two fluxes are equal only for small density of the total one [1]. For the total energy of fluxes larger than some threshold value, the wave propagates mainly along one of the interfaces. All the possible localized solutions in such a system in the case of attractive character of interfaces and nonlinear medium outside them are found analytically and studied both analytically and numerically. We demonstrated that the exact solutions are governed by a single scaling variable which describes the ratio between the interface distance and the soliton state localization length.

The total number of elementary excitations in the system and its total energy are found analytically. We present these dependences as functions of the distance between the interfaces in the universal scaling forms valid for different values of the interface “power”. We obtain numerically a monotonous behaviour of the reduced total number of elementary excitations as a function of the scaling variable characterizing the distance between the interfaces.

Using the exact solution of the nonlinear Schrödinger equation on intervals of constant potentials opens the possibility to treat various problems of localization using the appropriate boundary conditions. The obtained results can be applied for the description of localization of nonlinear wave fluxes in multilayered systems of different physical origin.

- [1] I. V. Gerasimchuk, A. S. Kovalev. Low Temp. Phys., 2000, 26, 8, 586-593.
- [2] I. V. Gerasimchuk, A. S. Kovalev. JETP Lett., 2007, 85, 10, 488-492.

LOCALIZATION OF NONLINEAR WAVES NEAR NONLINEAR INTERFACE

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The study of propagation and the character of localization of nonlinear waves in periodic and modulated systems on meso- and nanoscales is one of the main problems of the dynamics of nonlinear waves and solitons. The model describing an optical waveguide consisting of both linear and nonlinear parts, in a linear medium, was introduced by Malomed et al. [1]. The instability of the soliton state supported by a purely nonlinear defect, and a possibility to stabilize it by linear potentials were demonstrated in [2].

In this work in the framework of the investigation of wave localization in systems with Kerr nonlinearity in optical waveguides, we study the localization of soliton states near a single nonlinear waveguide (interface) and describe all possible localized modes in such a system. Because of the wave localization in a plane waveguide (or localization of oscillations at the interface) there nonlinear properties appear. We take into account the Kerr nonlinearity only in the waveguides (assuming that the width of the waveguides is much smaller than the distance between adjacent ones), and describe the waveguides by both nonlinear and linear terms. The medium between the waveguides is assumed to be optically linear.

We demonstrated that the soliton states localized near the nonlinear waveguide are possible for any sign of anharmonicity in the case of attraction of elementary excitations to the waveguide. However, for the mutual repulsion between the elementary excitations inside the waveguide, the localized states can exist only in the case of attractive character of the waveguide. That is, localized states near attractive waveguide are possible even for a repulsive character of interaction between the excitations inside the waveguide. For all possible localized states, the total number of elementary excitations and the total energy of the system were found and analyzed.

The present study can be useful for a wide range of physical applications: in nonlinear dynamics of solids, photonic and magnonic crystals, modulated (layered) media with a periodic system of nonlinear waveguides (interfaces or defect layers), Bose-Einstein condensation, magnetic multilayers with an array of plane magnetic defects, etc.

References

- [1] B. A. Malomed, M. Ya. Azbel. Phys. Rev. B, 1993, 47, 16, 10402.
- [2] N. Dror, B. A. Malomed. Phys. Rev. A, 2011, 83, 3, 033828.

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The first attempt at scientific study of the phenomenon occurring in matter - Thermodynamics, in spite of considering the substance as a continuous substance, gave a definite impetus to the development of technology, but could not explain many phenomena observed by that time. It became necessary to turn to new concepts that considered the substance at the molecular-atomic level – Molecular-Kinetic Theory (MKT), which determined the most powerful development of different technologies. We can say that almost everything created by humans around us is based on MKT. But over past 40 – 50 years experimental data have been accumulated, which MKT is unable to explain even qualitatively, observed in substances not only of nanoscale size but also of conventional dimensions and in the case of cryogenic temperatures, it is completely powerless. This clearly indicates that in order to eliminate this shortcoming, it is necessary to turn to new physical concepts. We propose new ideas for studying matter at a more precessional-electron level – Molecular-Potential Theory (MWT), which takes into account the state of chemical bonds between atoms and molecules during the passage of the entire phenomenon. As it is known, the electrons participating in the creation of chemical bonds can be in two quantum states: the bonding state and the antibonding state. These states are described by the corresponding energy levels, which in condensed media are combined into a bonding and antibonding energy zones. The electron in the antibonding zone and the hole in the bonding zone are antibonding quasiparticles (AQP). The transfer of an electron from the bonding zone to an antibonding site means the formation of an AQP that weakens the chemical bonds between the atoms around which it appears during its chaotic motion facilitating the change in the location of the atoms. The concentration of AQP can be varied as by the temperature as by the athermic pathway, as well as by a decrease in the dimensions of the sample in the nanoscale size. The latter opens up new technological opportunities. Examples are given confirming the conclusions listed above.

As it is known, the striking feature of the nanoworld is that all the characteristic properties of a substance on a nanosize scale depend on their size, in contrast to the material of larger sizes for which they are constants [1, 2]. This opens up tremendous opportunities for the creation of new nanotechnologies in any field of human activity, as in the positive as in the negative sense. But this raises the question for researchers: are the phenomena observable in nanoscale substances subject to the already known laws of nature, or do they cast doubt on previous ideas about physics. The nanosize scale of matter is also interesting because in this field in different cases it is possible to apply representations of both classical physics, in the form of Molecular-kinetic theory, and quantum physics. But as it turned out to date Molecular-Kinetic Theory (MKT) [3] is unable to explain many of the observed phenomena, not only in nanoscale but also in substances of ordinary size. This played, probably, an important role in the fact that in recent years the number of publications dealing with nanophysics and nanotechnology has decreased. Let us give some examples of the insolvency of MKT: 1) the mechanism of phase

transitions[4], 2) diffusion in solid and liquid [5], 3) dimer, trimer of atoms in steam, 4) increase viscosity with temperature[6], 5) curing of gas under the action of light, etc. And in the case of a phenomenon associated with a change in the location of an atom at low temperatures, it is completely powerless to explain the observed phenomenon [7].

In this paper, based on experimental data, we tried to prove that in both cases the same laws apply, if we apply new more processional concepts of the nature of the substance than is the case in MKT. New ideas, in contrast to MKT, take into account the state of chemical bonds between neighboring atoms under given conditions (Molecular-Potential Theory (MPT)) and explain all the phenomena in matter related to the change in the location of the atom in it [7].

Firstly, let us talk a little about the ways of development of natural science. People watching certain phenomena try to use them and understand their essence. To do this, based on the knowledge available for that time and intuition, models are created, changing with increase in the knowledge, etc. For example, first of all, the science of matter considered it as a non-separate substance and thermodynamics was created, which gave a powerful impetus to the development of science and technology. But over time it turned out that it was powerless to explain the observed new phenomenon. It became necessary to recognize that the substance is discrete and MKT [3] was created, which gave a more powerful impetus to the development of science and technology. It is possible to say with confidence almost everything that surrounds us is created on the basis of MKT. However, with the growth of experimental data, more and more results appeared that could not be explained on the basis of MKT. Here are some examples of the insolvency of MKT that are usually ignored.

1) There is no mechanism for a first-order phase transition (**Figure 1**) at the atomic level. To confirm this, we give the opinion of the famous scientist Goodstein: “melting and boiling – at first glance, easily understandable phenomena lead to a dead end of scientists, because until now there is no satisfactory explanation at the microscopic level” [4].

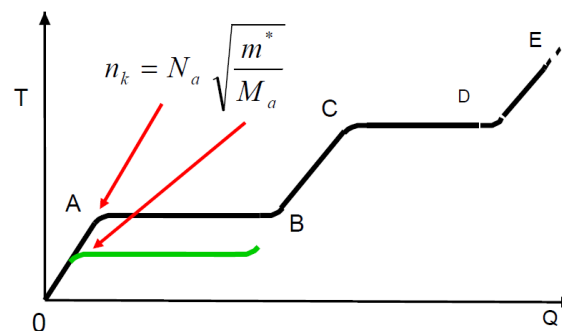


Figure1. Dependence of substance temperature on amount of heat transferred.

2) It is known that the values of the self-diffusion coefficients of all chemical elements at temperatures approximately equal to their melting point in the solid and liquid state strongly differ by several orders of magnitude for each element [5] (see **Figure 2** and **Table 1**).

As it is well known, the thermal coefficient of diffusion is determined by the expression

$$D = D_0 \exp(-U/kT). \quad (1)$$

where U is the activation energy of diffusion, usually of the order of eV, T is the temperature of diffusion, k is the Boltzmann constant, D_0 is weakly dependent factor temperature [5]. Since the temperature can be assumed to be the same, an increase in the coefficient of self-diffusion is due to a decrease in the activation energy U . It is clear that the chemical bonds force has decreased. But why at the same temperature the strength of the chemical bonds has decreased?

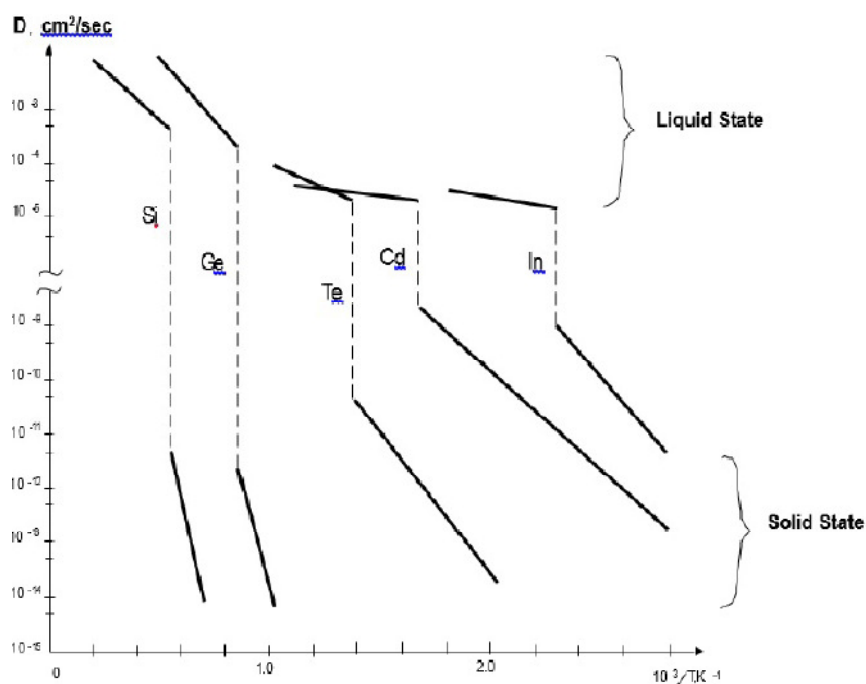


Figure 2. Temperature dependence of self-diffusion coefficients of elements in solid and liquid states.

Table 1. Coefficients of self-diffusion of elements in solid and in liquid states.

#	Element	Melting Temperature T , K	Diffusion coefficient in solid state, D , cm^2 / s	Diffusion coefficient in liquid state, D , cm^2 / s
1	Li	454	$9.4 \cdot 10^{-8}$	$6.6 \cdot 10^{-5}$
2	Na	371	$2.4 \cdot 10^{-7}$	$3.6 \cdot 10^{-5}$
3	Cu	1356	$5.4 \cdot 10^{-8}$	$2.6 \cdot 10^{-5}$
4	Ag	1234	$5.2 \cdot 10^{-9}$	$2.4 \cdot 10^{-5}$
5	Au	1336	$5.4 \cdot 10^{-9}$	$2.1 \cdot 10^{-5}$
6	Mg	923	$2.6 \cdot 10^{-8}$	$6.0 \cdot 10^{-5}$
7	Al	933	$1.6 \cdot 10^{-7}$	$7.2 \cdot 10^{-5}$
8	Cd	594	$6.0 \cdot 10^{-9}$	$1.8 \cdot 10^{-5}$
9	Tl	577	$1.2 \cdot 10^{-9}$	$1.6 \cdot 10^{-5}$
10	Sn	505	$3.4 \cdot 10^{-11}$	$6.3 \cdot 10^{-5}$
11	In	430	$9.5 \cdot 10^{-10}$	$1.6 \cdot 10^{-5}$
12	Pb	600	$3.6 \cdot 10^{-10}$	$4.6 \cdot 10^{-5}$
13	Si	1683	$5.6 \cdot 10^{-12}$	$1.9 \cdot 10^{-4}$
14	Ge	1210	$1.1 \cdot 10^{-12}$	$1.7 \cdot 10^{-4}$
15	Sb	904	$1.9 \cdot 10^{-10}$	$3.8 \cdot 10^{-5}$
16	Te	723	$6.0 \cdot 10^{-11}$	$3.1 \cdot 10^{-5}$
17	Fe	1803	$2.0 \cdot 10^{-7}$	$2.7 \cdot 10^{-5}$
18	Co	1765	$1.4 \cdot 10^{-9}$	$4.0 \cdot 10^{-5}$

In addition, the values of the coefficients of self-diffusion of all chemical elements in the solid state also differ greatly for different elements, whereas in the liquid state this difference is only one or two orders of magnitude (**Table 1**). It should be noted that the coefficient of diffusion of impurity atoms under the light stimulated (above certain intensities) diffusion is orders of magnitude greater than in the case of thermal diffusion at the same temperatures. This difference decreases with increasing of the temperature.

3) It turned out that, when the mass spectrometer was examining the composition of the equilibrium vapor present over the melted chemical element at temperatures just above T_m , the vapor consists of the single atoms of the element, but with increasing T , dimer appears, with a further increase in temperature, trimers appear, and so on, forming the clusters consisting of 7 to 10 atoms (**Figure 3**). If the vapor is formed due to the fact that at T_m the kinetic energy of the atoms is already able to rupture the chemical bonds and divide the atoms, turning the liquid into vapor, why they again begin to unite with increasing in the temperature, i.e. in the kinetic energy of the atoms? MKT is unable to explain this!

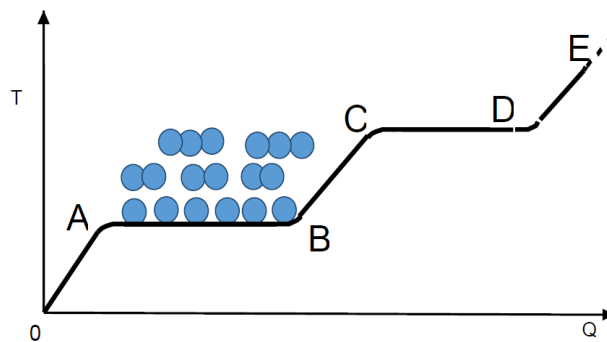


Figure 3. Increase in number of connected atoms in equilibrium vapor with increasing in temperature.

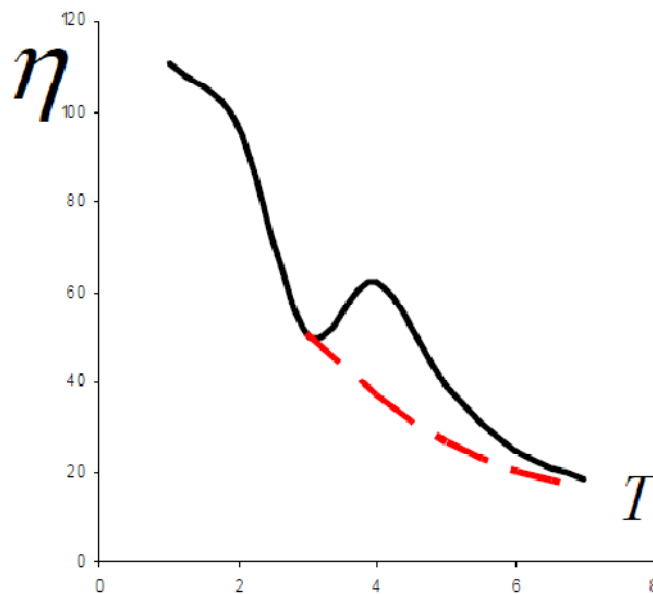


Figure 4. Temperature dependence of substance viscosity.

4) It is known that the viscosity of a substance decreases with increasing in the temperature, which, naturally, is associated with an increase in the kinetic energy of atoms, which reduces the chemical strength of connection. But for some substances after a decrease, in a certain temperature range the viscosity increases and then decreases again (Figure 4).

5) An experimental fact is known, which is hardly discussed in the scientific literature. In one part of the sealed transparent ampoule a solid substance (GaAs) is located. The ampoule is placed in the heater and its middle part can be illuminated (**Figure 5**). As a result of heating, the solid substance sublimates filling the entire ampoule with steam. During illumination, the particles of the condensed matter fall out. Thus, when the electromagnetic energy is added to the kinetic energy that sublimates the substance, its condensation takes place!

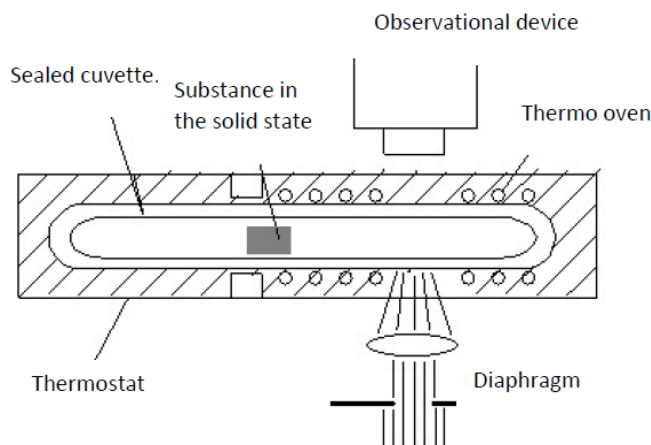


Figure 5. Gas curing due to lighting.

All this clearly indicates that it is necessary to correct or improve the theory. We propose new more precessional concepts for explaining all the phenomena associated with a change in the location of an atom in condensed media, both at high and low temperatures. Unlike MKT, which considers matter only at the atomic-molecular level, we also consider it at the electronic level and show that all physicochemical properties are determined by the electrons participating in the creation of chemical bonds between atoms.

The main provisions of MKT are as follows: 1. All bodies consist of a large number of smallest particles (atoms, molecules or ions). 2. The particles forming the body continuously and randomly (chaotic) move. 3. The forces of attraction and repulsion act between the particles forming the body. But it does not specify how this is done and requires the use of idealized and simplified assumptions about the motion and interaction of molecules (for example: molecules are considered as elastic nuclei, etc.), which incorrectly describes the properties of a real body. Therefore, we replaced item 3 in the following way: all interactions between particles that make up the body are determined by the state of their electrons involved in creating chemical bonds between them.

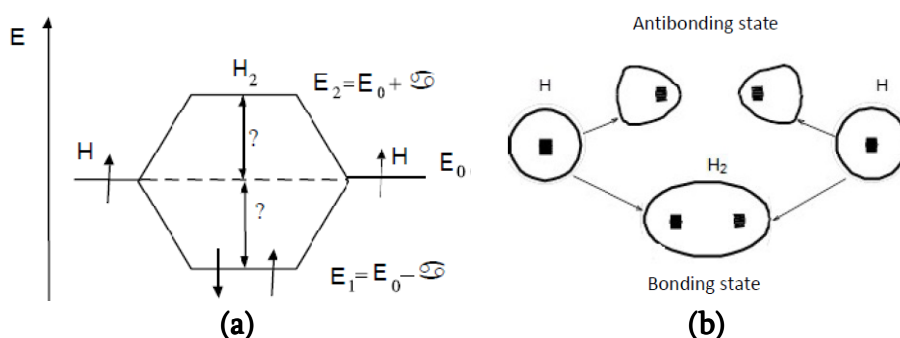


Figure 6. (a) Population of the energy levels of two atomic molecules by electrons of constituent atoms. (b) Distribution of negative charge density at binding and antibonding levels.

To facilitate the perception of our presentation (our report), let us recall some well-known issues (positions) about chemical bonds. When two atomic molecules are created (in the simplest case of identical atoms), the number of quantum states is preserved, but they are split into a bonding (with less than the initial energy) and an antibonding (with more than the initial energy) levels, on which the electrons are located, taking into account the Pauli principle and rules of Hund (**Figure 6**).

Two atomic molecules are divided into three groups, depending on how the energy of the chemical bond changes, when they take one electron, i.e. they are once ionized. In one group, the energy of the chemical bond decreases, while in the second increases (!). And the third does not change the rice.

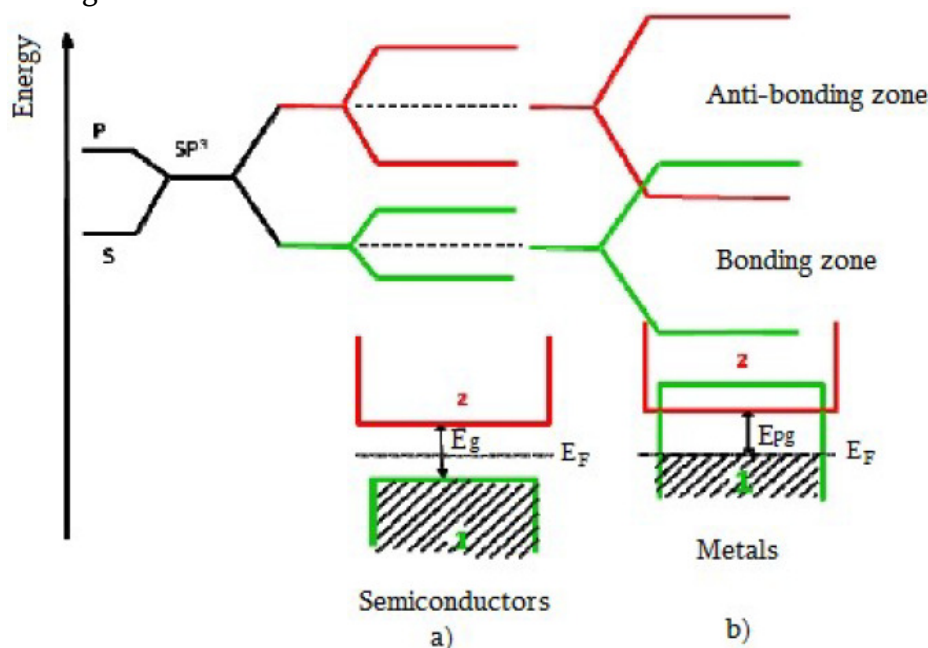


Figure 7. During the approach of atoms the formation (on the example of IVGroup of Periodic System) hybridized orbitals and their further splitting on binding and anti-binding orbitals of which with further approach of the atoms are formed bonding and anti-binding zone. Bonding and anti-binding energy bands: a) semiconductor or dielectric, b) metal, where E_F is the Fermi level, E_g is the band gap in semiconductors and E_{pg} is the pseudo-gap in metals.

Thus, the electrons participating in creating a chemical bond can be in two states, being in one state they strengthen the connection and in the other – weaken it. In the language of quantum mechanics, the first is called the bonding state (the bonding orbital), the second is called the antibonding state (the antibonding orbital). And the electrons located on these orbitals, i.e. energy levels are called, respectively, bonding and antibonding electrons, the ratio of the number of electrons located at these energy levels near a given atom determines the force (energy) of the chemical bond with neighboring atoms [8]. The more electrons are at the bonding energy levels, in comparison with those located on antibonding, the greater is the energy of the chemical bond. If these quantities are equal, then the chemical bond energy is zero (that is, there is no chemical bond and the substance passes into the gaseous state), since the energy gain of the system due to bonding electrons (minimum energy) is leveled by antibonding electrons (maximum energy). In solid bodies (consisting of a large number of atoms), bonding and antibonding states are transformed into corresponding zones of a certain energy width [8]. In dielectrics and semiconductors, these zones are separated by an energy gap, the so-called “forbidden band”, and in metals they are blocked by pseudo-gap **Figure 7**.

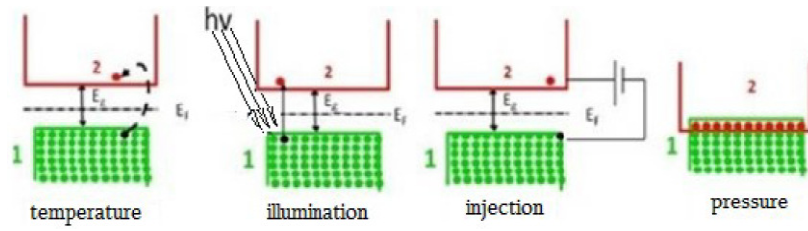


Figure 8. Methods of formation of AQP.

So, the structure of the energy bands of substances, their mutual location on the energy scale and their filling with electrons, at a given temperature and external conditions, completely determine all the properties of these substances. Their change as a result of any influence (temperature, pressure, light, different fields) causes a change in the various properties of substances (aggregate state, conductivity, mechanical and optical properties, etc. For example, Sn at low temperature is a semiconductor, at room temperature – a metal [9]). As a result of the transition of the electron from the bonding to the antibonding zone, an electron appears in it, and a free space, the so-called hole, is formed in the bonding zone. Both these quasiparticles decrease the energy of the chemical bond between the atoms around which they find themselves during their chaotic motion and, therefore, they can be called antibonding quasiparticles (AQP). Naturally, the greater the concentration of AQP, the weaker the chemical bond in the material and the easier it is to change the location of the atoms. It should be remembered that the AQP can be created both thermally and athermally (pressure, light, injection, magnetic and electric fields) **Figure 8**.

In the case of a solid body, if the AQPs are created in an athermal way, it must soften and expand with out heating (chemistry knows the rule: as the energy of the chemical bond decreases, its length increases, i.e. the distance between atoms [10]), which is proved experimentally [11 – 14]. Both experiments unequivocally prove the existence of AQPs and their affect on the increase in the probability W_A of the change in the location of atoms in matter. Based on the new representation of the MPT for the probability W_A of changing the location of atoms in matter, expression

$$W_A = A (n_{AQP} / N_a)^\beta W_{ph}, \quad (2)$$

where A is the constant value, n_{AQP} – the concent ration of the AQPs, N_a – the concent ration of the atoms (molecules) of the substance, the β – number of the AQPs of the given atom, required to reduce the height of the potential barrier to zero, W_{ph} is the probability of the presence of phonons of a certain energy near a given atom [15, 16].

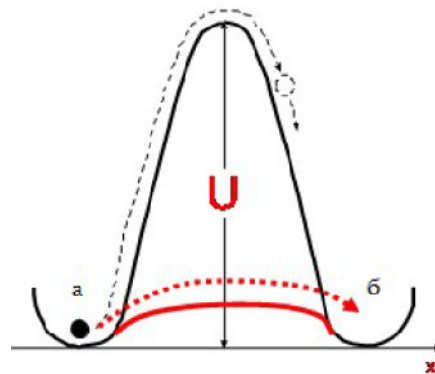


Figure 9. Schematic illustration of transition of atom from one location to another: a – according to MKT (U is height of potential barrier) and b – according to MPT.

Starting from MKT, for the transition of an atom from one location to another, it is necessary to get a fluctuation of the kinetic energy sufficient for breaking chemical bonds by neighboring atoms, described in MKT by the height of the potential barrier (Figure 9a). The probability W_A of this transition is expressed by the relation

$$W_A = B \exp(-U/kT), \quad (3)$$

where U is the height of the potential barrier (the energy of the chemical bond of the given atom is neighboring), T is the temperature, k is the Boltzmann constant, B is a coefficient that weakly depends on the temperature. New mechanism requires a lowering of the height to fit the potential barrier (Figure 9b) such a change in the state of chemical bonds, which will reduce their energy, which is due to the appearance of the AQP's about a given atom with probability (2). It is seen from this formula that W_A does not depend on temperature, in contrast to (3), which has an exponential temperature-dependence. Thus, it is clear that the MKT mechanism is valid only at high temperatures in comparison with the second mechanism of MPT, which works also at low temperatures in the case of athermal effects on the test material [11 – 14]. Let us give an explanation of the above incomprehensible phenomena.

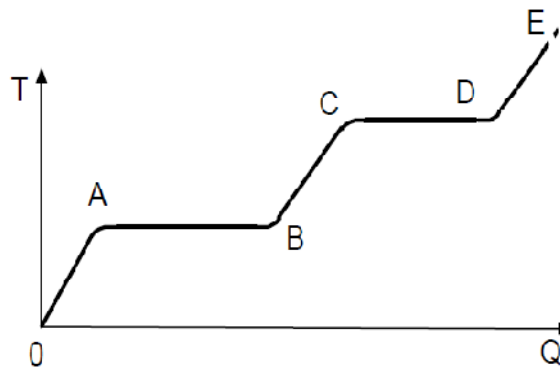


Figure 10. Dependence of substance temperature on amount of heat transferred to it

The graph of the dependence of the temperature of the substance on the transmitted heat (Figure 10) shows that the temperature of the substance increases with the increase in the amount of heat transferred to a certain temperature (T_m is the melting point) (section OA), after which it ceases to change (section AB) that the transfer of heat (kinetic energy) continues. In this case, the substance at point A is in a solid state, and at point B is already liquid, while the temperature at both points is the same. It is believed that in the region corresponding to the section AB, at which the temperature does not increase, the kinetic energy transferred to the substance in the form of heat is expended on the rupture of chemical bonds [6]. But it was experimentally established that the energy of the chemical bonds at points A and B differs from each other by only 5 – 10 %, and by X-ray diffraction analysis it was shown that at point B the short-range order (i.e. certain positions of neighboring atoms near a given atom) is not violated, But there is already a mechanical instability of the substance (a sharp decrease in shear resistance, an increase in fluidity). Because of this contradiction, it is very important to consider in more detail the processes that occur when heat is transferred to a substance. At the beginning (OA section) as a result of heat transfer, the kinetic energy of the substance increases i.e., its temperature. The heat transmitted to the matter propagates in it in two subsystems: atomic (heavy) and electronic (light). Simultaneously, there is a transition of electrons from the bonding to the antibonding zone. Each transition corresponds to the appearance of an electron in the antibonding zone and holes in the bonding zone. This changes the potential energy of the

electron and the distribution of its probability of being in space, i.e. the spatial distribution of its density. From an acute directed P state to an isotropic S state [17].

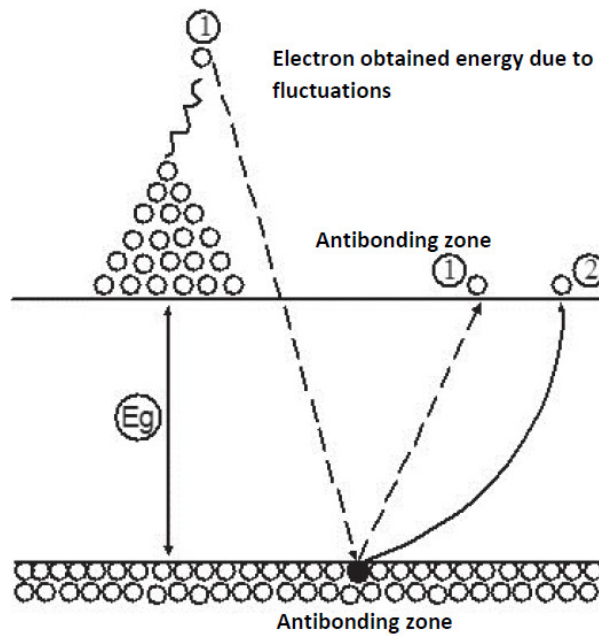


Figure 11. A schematic representation of transfer of electron from bonding zone to antibonding by electron–electron collisions (impact mechanism): 1 –electron colliding with bound electron and passing into antibonding zone and 2 – electron released by impact mechanism.

The transition of electrons from the bonding to the antibonding zone can occur in two ways: 1) the fluctuation of the kinetic energy of the atoms formed as a result of their collision (a heavy subsystem), 2) the fluctuation of the kinetic energy of the electrons formed as a result of their collision (the light subsystem), the so-called impact mechanism [7], **Figure 11**. Because of the chaotic motion of the electrons, with some probability, an electron may have more energy than the forbidden band E_g as a result of the fluctuation, and when this electron collides with the bound electron it transfers energy to it, liberates it, and “cool down” the same remains in the antibonding zone (**Figure 11**). Thus, the kinetic energy was converted into a potential energy so that the kinetic energy of the atoms remained unchanged. At the initial stage, despite that free carriers-AQP are much lighter than atoms and their velocity at a given temperature is much larger, the probability of the first process prevails over the second, since the concentration of atoms is of the order of 10^{22}cm^{-3} , and the concentration of AQP is many orders of magnitude less. But as the temperature rises, the concentration of AQP increases and the probability of the second process increases. As a result of AQP, an increasing proportion of the kinetic energy received as heat is spent on the formation of new AQP. After reaching the melting temperature T_m , the heat transferred to the material no longer causes an increase in temperature due to the fact that the transferred kinetic energy (the heat transfer rate) is compared with the spent kinetic energy for creating the AQP by the impact mechanism. In the case when the heat transfer rate is greater than the rate of its waste, the substance overheats, and with the reverse ratio of the rates, subcooling occurs. Since the fluctuations in matter are spatially inhomogeneous, in some regions of the material melting will start earlier. The amount of heat carried by the atomic subsystem per unit time is $kTn_a v_a$, and the transferred AQP will be $kTn_e v_e$, where kT is the average kinetic energy per particle (atom or AQP), n_e and N_a ,

respectively the concentrations of AQP and atoms, and v_e and v_a are their average thermal velocities. Since $v_e > v_a$, a smaller concentration of AQP than atoms is required to transfer the same amount of heat. The determination of this concentration is possible from the equation: $kTn_c v_e = kTN_a v_a$. This equality occurs at the melting temperature T_m , and n_c is the critical concentration. Below T_m , $kTn_c v_e < kTN_a v_a$ and for $T_m - kTn_c v_e = kTN_a v_a$. In this case, the probability of a fluctuation with an energy greater than E_g in the AQP subsystem is greater than in the atomic subsystem, due to the fact that $v_e > v_a$.

Let's calculate, say for Si, the concentration of AQP necessary to ensure that all transferred heat is redistributed between the AQP, so that there is nothing left for the atoms. This will happen in the event that during the time of a single oscillation of an atom near each atom, which has received additional kinetic energy, will necessarily turn out to be an AQP and take this additional kinetic energy. This energy will quickly redistribute between the AQP and create a fluctuation with energy, more than necessary for the formation of a new AQP by the impact mechanism [18]. In this case, due to the excess energy, the impacting AQP continues to exist, thereby increasing the concentration of the AQP, which leads to a decrease in the bonding energy between the atoms, i.e. change in potential energy. Thus, the kinetic energy was converted into a potential energy, so that the kinetic energy of the atoms did not change. We will estimate the concentration of the AQP necessary to make this happen. During the time of a single oscillation of the atom $\tau \approx 5 \cdot 10^{-13}$ s, the AQP which velocity, at T_m is $v \approx 5 \cdot 10^7$ cm / s, will pass the distance $s = v \tau \approx 2.5 \cdot 10^{-5}$ cm. If we divide this value by the interatomic distance, we obtain the number of atoms that will run through the AQP for a time τ that is ≈ 1000 . Therefore, in order for all $5 \cdot 10^{22}$ cm⁻³ atoms to appear during the time τ , $\sim 10^{19}$ cm⁻³ AQP is necessary. The same value is obtained from the formula $kTn_c v_{AQP} = kTN_a v_a$ if we substitute in it the average values of the velocities of thermal motion: for AQP, $m^* v_{AQP}^2 / 2 = 3kT/2$ (where $v_{AQP} = (v_e + v_h)/2$), and for atoms $M v_a^2 / 2 = 3kT/2$. From this we get: $n_c = N_a (m^* / M_a)^{1/2}$, where m^* is the average conductivity mass of an electron and a hole, M_a is the mass of an atom, N_a is the concentration of atoms. The concentration of n_c , upon which all the heat transferred to the substance is spent on the formation of new AQP is called critical concentration. Each substance has its critical concentration n_c (for example, for Si – $6 \cdot 10^{19}$ cm⁻³, for Ge – $2 \cdot 10^{19}$ cm⁻³, for GaAs – $4 \cdot 10^{18}$ cm⁻³), the values calculated by both methods coincide with the concentrations of AQP, measured experimentally at a temperature very close to the melting temperature T_m . This means that to start the melting process, the critical concentration n_c , rather than the temperature, is the main one. If n_c is formed by some athermal method, then the melting process will begin at $T < T_m$, which is confirmed experimentally. In the region of the AB curve shown in **Figure 9a**, all transmitted heat is spent on the formation of new AQP (i.e. ionization of the atoms takes place in the sense that the electron is taken from the chemical bond and the electron is transferred to the antibonding zone), so their concentration increases. If at point A it was $\sim 5 \cdot 10^{18} - 10^{19}$ cm⁻³ then in point B it reaches $\sim 5 \cdot 10^{21} - 10^{22}$ cm⁻³ and this means that on $\sim 5 - 9$ non-ionized atoms there is already one ionized atom. Then the probability of transferring the kinetic energy to the ionized atom increases, and since much more energy is required for secondary ionization, secondary ionization does not occur and the kinetic energy is transferred to the vibrations of the atom, which means a gradual increase in temperature, as the number of ionized atoms (the BD region). After point B, as the temperature increases, the bonding and antibonding bands continue to move along the energy scale to each other [11], so the secondary ionization energy decreases. Then, when the rate of secondary ionization is equal to the rate of arrival of the kinetic energy, all the energy entering the substance will be spent on the

formation of the AQP and the temperature will cease to grow. In the case of the double ionized atom of four valence electrons two electrons will be at the bonding level and two on the antibonding level, but this means that it does not have a connection with neighbors. A rudimentary gas is formed. With the growth of these gas spheres, opalescence will occur and then boiling. Thus, an important conclusion follows: processes usually carried out at high temperatures can also be carried out at low temperatures!

The value of the coefficient of diffusion is the greater the probability of the W_A change in the location of the atoms in the substance, which, as mentioned above (2), is determined by the concentration of the AQP. It is several orders of magnitude higher in the liquid state than in the solid state (at the melting point in the solid state (point A in **Figure 10**), the concentration of AQP is of the order of $5 \cdot 10^{17} - 5 \cdot 10^{19} \text{ cm}^{-3}$ and in liquid $5 \cdot 10^{21} - 10^{22} \text{ cm}^{-3}$ (point B, Figure 10). Therefore, the values of the coefficients in the solid state are several orders of magnitude smaller than in the liquid state. As to the small difference between the values of the self-diffusion coefficients of all chemical elements in the liquid state, the concentration of the AQP for all elements is almost the same for the preparation of a liquid state, of the order of 10^{22} cm^{-3} . If, at low temperatures, creating an AQP concentration being more than equilibrium one at a given temperature by the athermic method (for example, light), the value of the photostimulated diffusion coefficient will be larger than the thermal. It should also be shown here that MKT is a particular case of MPT suitable only at high temperatures of the order of approximately $T = 0.7 T_m$ (T_m is the melting point). Indeed, according to the MKT, the diffusion coefficient has the form $D = D_0 \exp(-U/kT)$, and for MPT

$$D = D_1 (n_{AQP} / N_a)^6 W_F, \quad (4)$$

where D_1 , just like D_0 , depends weakly on temperature. In the case of thermal diffusion, AQP are formed by temperature and the concentration of AQP is expressed by the formula[6]:

$$n_i = (N_c N_v)^{1/2} \exp(-E_g / kT). \quad (5)$$

If in (4) instead of n AQP insert (5) then a traditional MKT formula is obtained for the thermal diffusion coefficient (1), in which the activation energy is $U = \beta E_g$, which unequivocally proves that MKT is a special case of MPT.

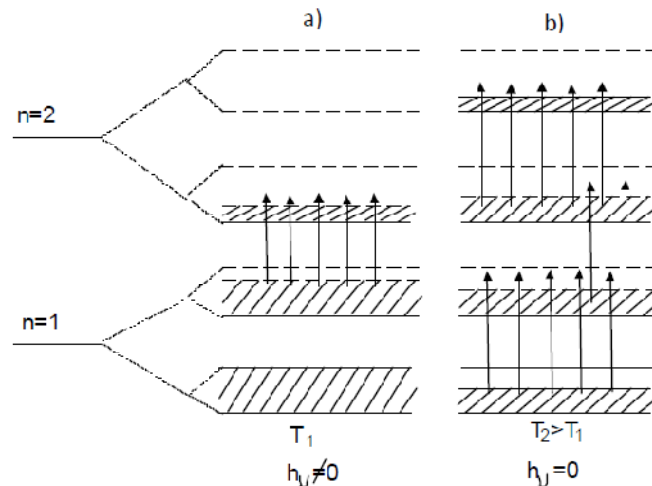


Figure 12. Location of energy bands in case of principal quantum numbers $n = 1$ and $n = 2$. Transitions of electrons: a) as a result of the influence of temperature and/ or light, excess of electrons is created at binding levels for quantum numbers $n = 1$ and $n = 2$ and energy of chemical bond increases and b) as result of influence of temperature, excess of electrons is created at antibonding levels for quantum numbers $n = 1$ and $n = 2$ and energy of chemical bond decreases.

In order to explain the phenomenon described in points 3, 4 and 5, it is necessary to return to the energy structure of the substance and take into account the levels with the quantum number $n = 2$. It is seen from **Figure 12a** that when the atoms approach each other, these energy levels, like for $n = 1$, split into bonding and antibonding levels and then into zones. The transfer of an electron from the antibonding level for $n = 1$, by bonding for $n = 2$, increases the energy of the chemical bond. In the case of the formation of atomic clusters in an equilibrium pair with increasing temperature (point 3), the electron is transferred by temperature. In the case of curing the steam under lighting (point 5), the electron is transferred by light. Increase in viscosity with increase in temperature in a certain temperature range and then the decrease (point 4) is easily explained by the electron transitions shown in **Figure 12b**.

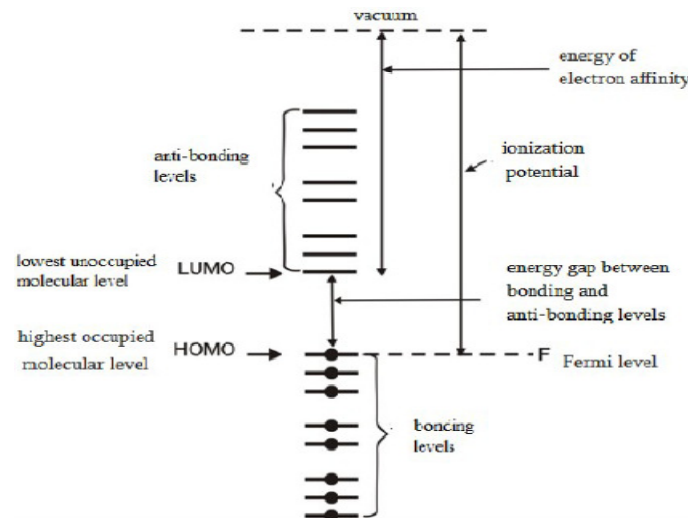


Figure 13. Energy structure of nanoparticle. HOMO – Higher Occupied Molecular Orbital (level) and LUMO – Lower Unoccupied Molecular Orbital (level). I – ionization potential and Q – energy of electron affinity.

A new mechanism for changing the location of an atom is also valid for nanoparticles, despite their electronic structure having a discrete character (**Figure 13**) with bonding and antibonding levels in it. An electron translated in some way into antibonding levels will move freely at these levels, if between levels the energy distance of the order kT is, which is realized at room temperature.

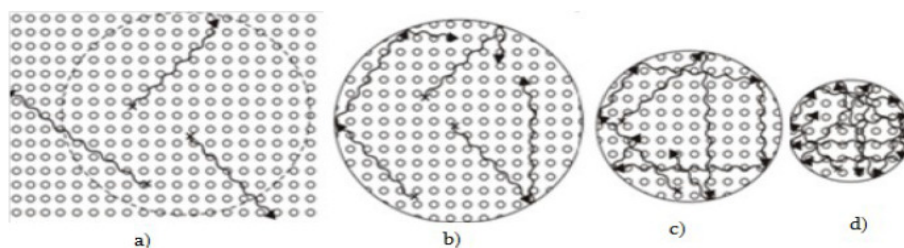


Figure 14. Schematic illustration of growth in AQPs' concentration with reducing in nanoparticles size at given temperature. Increasing in ABQPs effective concentration for fixed real concentration with decreasing in sizes: a) ABQP trajectory in compact solid's region with volume equal to nanoparticle volume: two of them are leaving volume; b) in connection with the reflection from boundary surface of nanoparticle trajectory three ABQP is in it and they will be around more number of atoms in this volume than in case of a compact solid body; c) and d) with decreasing size of nanoparticles of the same three ABQP will be near a larger number of atoms.

The change in the concentration of AQP, in addition to exposure to traditional athermic methods, can also be a change in the size of the substance (**Figure 14**).

The account of the effective concentration explains all the “anomalies”, which arise in nanoparticles with a decrease in their size.

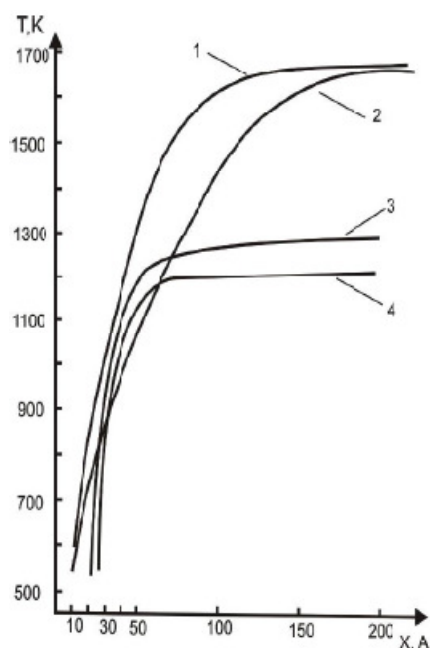


Figure 15. Dependence of melting temperature of nanoparticle as function of its size. 1) For the entire Si nanoparticle. 2) Only for surface of Si nanoparticles. 3) Experimental data for entire Au nanoparticle. 4) Theoretically calculated data for entire Au nanoparticle.

Let's give some examples. **Figure 15** shows the dependence of the melting temperature of nanoparticles on their size, from which one can see that the decrease in the size of the nanoparticles decreases the melting point. To explain this interesting phenomenon, let us recall the above reasoning: in AQP nanoparticles, the chemical bonds weaken more than in a compact solid, which is quantitatively taken into account in the notion of effective concentration. It was also noted that with an increase in the size of nanoparticles, the effective concentration increases and that the probability of the presence of AQP in surface layer atoms is greater than that of atoms in the inner region due to reflection from the surface. This leads to a softening of the surface layer. It is shown that the melting of a solid begins after reaching a critical concentration of the AQP, and the concentration is critical when the AQP has time to come to all atoms in the period of a single oscillation of the atom and take the additional energy of the vibration of atoms that it received from outside as heat. The effective concentration rises to a critical value at a low real concentration the smaller is the size of nanoparticles. A low real concentration is achieved at lower temperatures than the melting point, but the total concentration with the effective concentration can reach a critical value, which will initiate the melting process. Proceeding from this, the smaller is the size of the nanoparticle, the lower is the temperature, it begins to melt, and the melting of the surface layer starts earlier. Therefore, at a certain temperature, a nanoparticle state is obtained when its surface is molten, and the inner part is solid. The curve of the dependence of the melting temperature on the dimensions of the nanoparticles, calculated using the effective concentration of the AQP, is shown to be in good agreement with the curve constructed from the experimental data.

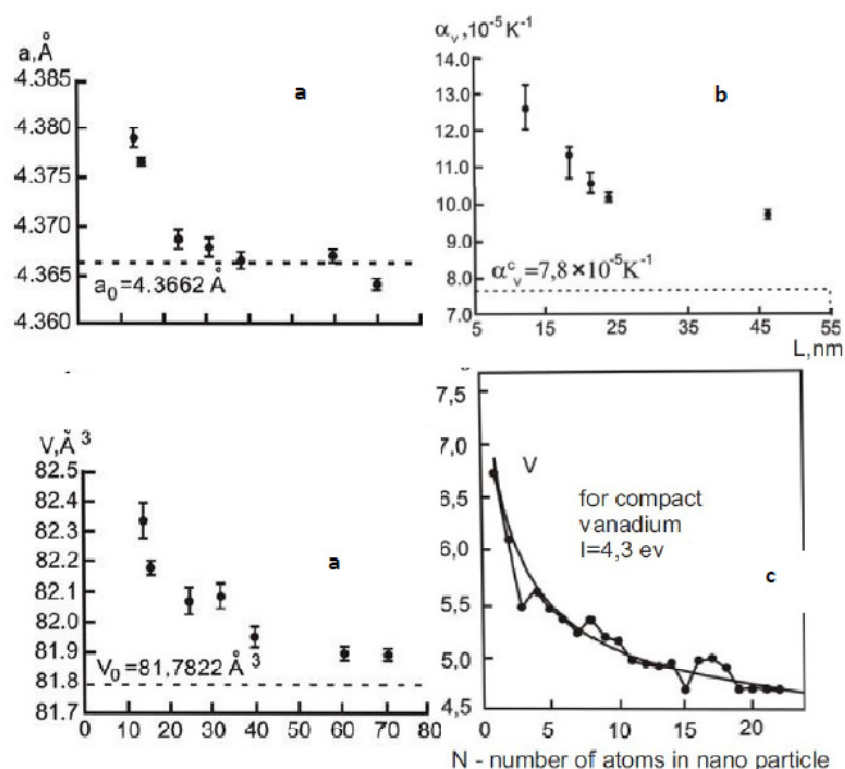


Figure 16. Dependence of values of fundamental parameters on nanoparticle sizes. a) Lattice parameter and volume of unit cell V ; b) thermal expansion coefficient of Se; and c) Ionization potential I .

Thus, it is unambiguously shown that taking into account the influence on the attenuation of chemical bonds of the effective concentration of AQP appearing at decrease in the size of nanoparticles well describes the quantitative dependence of the melting temperature on the size of nanoparticles and all the “anomalies” of the characteristics of nanoparticles observed with a decrease in their size **Figure 16**, [19].

References

1. S. P. Gubin. What is a nanoparticle? Trends in the development of nanochemistry and nanotechnology. *Uspeki – Chem.*, 2002, 3, 23-31.
2. J. Ramsden. *Nanotechnology: An Introduction*, 2011, Elsevier, 296 pp.
3. J. I. Frenkel. *Statistical Physics*, 1948, Moscow – Leningrad, Acad. Sci. USSR, 760 pp.
4. D. Goodstein. The phonon atom effect. *Phys. Abroad A*, 1988, 1, 196-213.
5. Ed. D. Shaw. *Atomic Diffusion in Semiconductors*, 1973, London – New York, Plenum Press.
6. P. V. Pavlov, A. F. Khokhlov. *Physics of Solids*, 2000, Moscow, Higher School, 494 pp.
7. A. B. Gerasimov. Principles of the molecular-potential theory. In: *Cont. 2nd Int. Conf. “Nanotechnologies”*, 2012, Tbilisi, Nekeri, 160-170.
8. W. A. Harrison. *Electronic Structure and the Properties of Solids. The Physics of the Chemical Bond*. 1980, San Francisco, W. H. Freeman & Co.
9. *Physical Quantities (Reference Book)*, 1991, Moscow, Energoatomizdat, 418-420.
10. N. L. Glinka. *General Chemistry*, 2003, Moscow, 623 pp.

11. A. B. Gerasimov. Electron-hole mechanism of atomic motion in a solid state. In: Proc. 4th Int. Conf. Mater. Sci. Forum Vols., 1990, 65-66, 47-51.
12. A. B. Gerasimov. Fundamentals of Low-Temperature Technology of Production of Semiconductor Devices, 2005, Tbilisi: Tbilisi Univ. Press, 235 pp.
13. G. D. Chiradze. PhD Thesis, 1992, Tbilisi, Tbilisi State Univ.
14. A. B. Gerasimov, Z. G. Gogua, G. Z. Gogua. Physical mechanism of expansion of semiconductors under the light. Bull. Georg. Acad. Sci., 2005, 170, 1, 61-62.
15. A. Gerasimov, A. Bibilashvili, D. Buachidze, I. Lomidze, R. Kazarov, D. Kimeridze. The Physical Nature of the Size Dependence of Nanoparticles Melting Temperature. Bull. Georg. Acad. Sci., 2005, 172, 2, 233-236.
16. A. Gerasimov, M. Vepkhvadze. A New Mechanism for the Dependence of the Properties of Nanoparticles on Their Size, 2017, Tbilisi, Nekeri, 109 pp.
17. A. B. Gerasimov, A. P. Bibilashvili, G. D. Chiradze, N. G. Kutivadze, Z. G. Bokhochadze. The influence of isotropization of chemical bonds on anisotropy of photomechanical effect. Bull. Georg. Acad. Sci., 1998, 157, 3, 396-399.
18. S. M. Ryvkin. Photoelectric Phenomena in Semiconductors, 1963, Moscow, Fizmatgiz, 494 pp.
19. A. B. Gerasimov, G. D. Chiradze, Z. G. Gogua. Widening of Si under the impact of illumination. Ukr. J. Phys., 2006, 51, 8, 785-787.

PHYSICAL MECHANISM OF HEAT CAPACITY OF NANOMATERIALS

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The physical nature of the increase in the heat capacity of nanomaterials with a decrease in the sizes of their constituent nanoparticles has so far not been clear. This is due to the fact that the existing heat capacity mechanisms are not perfect, since they are not only quantitative, but also from a qualitative point of view, unable to explain many experimental facts. We have proposed a new physical mechanism for the heat capacity of solids, based on the consideration of redistribution of the kinetic energy received by a solid body into a potential (deformation of chemical bonds) and the kinetic energy of the system (temperature) due to a change in the energy of chemical bonds. The less energy of chemical bonds, the more likely they are to deform. With increasing temperature, the decrease in the energy of chemical bonds is due to the growing concentration of the resulting antibonding quasiparticles (AQP), which weaken the chemical bonds between the atoms around which they appear during their chaotic motion. AQP are electrons in the antibonding zone and holes in the bonding zone. The transfer of an electron by heat from the bonding to the antibonding zone with the formation of a hole in the bonding zone means the appearance of an AQP. The greater the concentration of AQP the less the energy of chemical bonds, the more likely they are deformed and the larger the increase in the fraction of the change in the potential energy in the kinetic energy received by the solid body. An increase in the share of potential energy causes an increase in the amount of heat necessary for heating the body by one degree, i.e. its heat capacity. It is shown that as the size of nanoparticles decreases, the effective concentration of AQP increases, which leads to an increase in the probability of deformation of chemical bonds and, correspondingly, to an increase in the fraction of potential energy. Specific examples confirming the truth of the proposed mechanism are given.

PROCESS OF RT: PATIENT-SPECIFIC QA

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The process of radiotherapy (RT) is complex and involves an understanding of the principles of medical physics, radiobiology, radiation safety, dosimetry, radiation treatment planning, simulation and interaction of radiation with other treatment modalities. Each step in the integrated process of RT needs quality control and quality assurance (QA) to prevent errors and to give high confidence that patients will receive the prescribed treatment correctly.

A patient-specific quality assurance program has been developed to facilitate the clinical implementation of intensity modulated radiotherapy (IMRT) delivered using a micro-multileaf collimator. The methodology includes several dosimetric tasks that are performed prior to the treatment of each patient. Film dosimetry is performed for each individual field and for the multifield composite plan. Individual field measurements are performed at a depth of 5 cm in a water equivalent slab phantom; The heterogeneity inserts of the phantom are 2 cm × 2 cm × 22 cm with absorption characteristics of water, brain, muscle, lung, breast, adipose tissue, bone, and liver.

Export of dose calculations from the treatment planning system is similarly specified. For the composite distribution, parameters from the patient plan are applied to an IMRT phantom, and the film is exposed in an axial orientation. Distributions are compared with the aid of software developed for the specific tasks. The measured and calculated dose distributions can be superimposed and positioned graphically using the move, rotate, and mirror tools, as well as by specifying isocenter coordinates and using fiducial marks. Horizontal and vertical profiles are available for analysis. Dose difference, distance-to-agreement, and γ index, the minimum scaled multidimensional distance between a measurement and a calculation point determined in combined dose and physical distance space, are calculated along a specified isodose line and displayed. γ provides an excellent measure of disagreement between measurement and calculation for complex intensity distributions. We specify 3 % dose difference and 3 mm distance as our scaling acceptability criteria. Absolute dosimetry for each composite plan is performed using an ionization chamber. To date, excellent agreement between measurements and calculations has been observed.

An integrated film dosimetry protocol was developed for dose calibration, calibration curve fitting, dose mapping, and profile / gamma analysis. Patient-specific quality assurance (PSQA) was performed for SRS / SBRT treatment plans, and analysis of the measurements and calculations. The purpose of patient-specific Quality Assurance program is the objective, systematic monitoring of the quality and appropriateness of patient care. Such procedure is essential for all activities in radiation oncology.

SILICON CARBIDE BASED MATERIALS WITH TUNABLE PROPERTIES

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Silicon carbide is widely known and used due to its extraordinary properties (e.g. hardness, thermal conductivity, mechanical strength, chemical stability and biological inertness). Therefore the SiC-based nanostructured materials (nano-SiC: nanoparticles, nanowires and porous SiC) ways of working-out silicon-based materials adopted for selected practical proposals seems to be an actual task. Here we summarize results of preparation and properties tuning of different nano- SiC nanomaterials and possible ways of their application.

Porous SiC with highly-ordered crystalline structure could be produced by electrochemical etching of highly doped ($\rho \sim 1 \text{ m}\Omega \cdot \text{cm}$, n-type) bulk polycrystalline 3C-SiC substrates [1]. Large surface area ($\sim 100 \text{ m}^2 / \text{g}$) and wide mesopores (15 – 50 nm) make electrochemically-derived pore-SiC prospective as a catalytic support. The morphological parameters of this por-SiC could be controlled by etching conditions and electrical conductivity of the initial substrate. Another interesting product of the SiC electrochemical dissolution is carbon fluoroxyde (CFO), an organic-based oligomeric substance with intense photoluminescence, which could be used for bioimaging due to its low toxicity and biocompatibility [2].

The mesoporous SiC with well-developed morphology (surface area up to $800 \text{ m}^2 / \text{g}$) could be obtained by “bottom-up” nanocasting approach consisted of by thermal decomposition of preceramic polymer (polycarbosilane) in space-confined media [3]. The crystalline structure of “nanocasting” pore-SiC is not well-ordered, however it could be significantly improved by addition of Ni complexes into the reaction mixture.

The nanoparticles of SiC produced by industry are normally larger than 20 nm in size and possess uncontrolled surface terminations. We found, that thermal oxidation followed by oxide removal allowed the NPs size reduction from 20 to 9.8 nm [4]. Procedures of chemical treatment, allowing to produce nano-SiC predominantly covered with carboxylic acid or hydroxyl (Si–OH / C–OH) and hydrosilic (Si–H) groups and further chemical functionalization (amination, hydrosilylation of alkenes, esterification) were developed to change the SiC polarity and dispersibility in with various media.

References

- [1] ACS Appl. Nano Mater., 2018, 1, 6, 2609-2620.
- [2] J. Phys. Chem. C, 2015, 119, 35, 20503-20514.
- [3] RSC Adv., 2016, 6, 10, 108828-108839.
- [4] Langmuir, 2017, 33, 47, 13561-13571.

ELECTROCHEMICAL BEHAVIOR OF BENZENEPOLYCARBOXYLIC ACIDS WITH DIFFERENT CONTENT OF NUMBER AND LOCATION CARBOXYLIC GROUPS IN VARIOUS SOLVENTS

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The aim of our investigation is study of influence of nature of solvents – water, ethanol and ethylene glycol on electrochemical behavior of nanoparticles of benzenepolycarboxylic acids, with a different number and location of carboxylic groups. Particularly, we studied: trimellitic acid (1,2,4-benzenetricarboxylic acid), trimezinic acid (1,3,5-benzenetricarboxylic acid), piromellitic acid (1,2,4,5-benzenetetracarboxylic acid), mellitic acid with six carboxylic groups (1,2,3,4,5,6-benzenehexacarboxylic acid). It is well known, that benzenepolycarboxylic acids of different structure are applied in medicine and pharmacology. It is known, that the adsorption ability of nanoparticles of that substances, which used in medicine, helps to penetration of them in the living organism. Therefore, we have studied the adsorption ability of trimellitic, trimezinic, piromellitic and mellitic acids in the double electric layer in various solvents. The establishment of the adsorption ability of these acids in double electrical layer depending on the location and amounts of carboxylic groups is of great interest, such as for electrochemistry as especially for medicine and pharmacochimistry. The adsorption degree of these acids was studied by the method of measuring the differential capacity of the double electric layer. For the study of influence of nature of solutions on electrochemical behavior of the indicated acids solutions, which have different physical properties - water, mono atomic alcohol – ethanol and diatomic alcohol - ethylene glycol were chosen. It is clear that the viscosity of the solvent has a significant effect on the behavior of nanoparticles in solution. The diatomic alcohol – ethylene glycol is about 20 times more viscous liquid than water ($\eta = 0.89 \text{ mPa}$ water, 1.074 mPa ethanol, and 19.17 mPa ethylene glycol) at the 20°C temperature.

Adsorption ability of the above mentioned acids was studied at the mercury electrode in 0.5 M NaClO_4 in different solvents by measuring the differential capacity (C) as a function of electrode potential (E) by means AC bridge (C , E -curves). In order to thoroughly study the electrochemical behavior of nanoparticles of these acids, on the base of experimental data by the Frumkin–Damaskin theory we calculated the following significant parameters, characterizing the processes, taking place in the double electrical layer in various solvents: attraction constant – a ; the value of maximum adsorption – Γ_m , mol m^{-2} ; adsorption equilibrium constant – B , l mol^{-1} ; standard adsorption energy – ΔG_A , kJ mol^{-1} , the values of the charge of the electrode surface – q , $10^{-2} \text{ A s m}^{-2}$. On calculation of basic parameters characterizing behavior of nanoparticles at the interface of mercury / solutions, it was established, that all above mentioned acids have adsorption ability of different degree in double electrical layer.

NANO IRON OXIDE FUMES

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A process was developed in the 1950s in Linz by the Austrian steel company VOEST by blowing oxygen together with powdered CaO into the molten bath by means of a lance. Due to the high temperature in the converter some iron vaporized and immediately oxidized outside the converter forming a thick cloud of red fumes of iron oxide nano particles. The dust problem was solved later by introducing electrostatic precipitators.

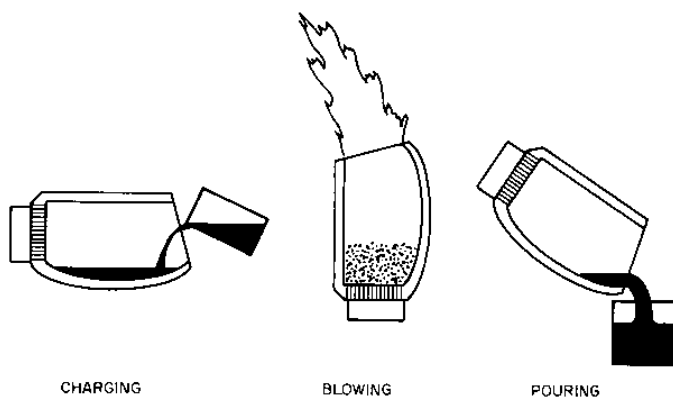


Figure 1. Sequence of operations in converter.



Figure 2. Converter during blowing period.



Figure 4. Location of Linz and Donawitz in Austria.



Figure 7. Celebrating 40 years LD at VOEST.

ACTIVATION VOLUME OF PLASTIC DEFORMATION OF ULTRAFINE-GRAINED COPPER

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In the last decades, many works have been devoted to the study of mechanisms that determine the unique mechanical properties of submicrocrystalline and nanocrystalline materials. However, the overwhelming part of the experimental investigations is restricted to a material at room temperature. The focus of the paper is on the thermal activation analysis based on stress relaxation experiments of such model material as copper in the temperature range 77 – 295 K. The oxygen-free copper (Cu-OF, 99.98 %) have been investigated in this study. Ultrafine-grained (UFG) microstructure of polycrystals was received by equal-channel angular hydroextrusion (ECAE) [1]. The grain size was 500 nm. The samples were deformed by tension with the constant strain rate of 10^{-4} s^{-1} . During the test, the stress relaxation measurements were carried out. The dependences of the flow stress $\sigma_\varepsilon(T)$ for a fixed deformation and the activation volume $V_a(T)$, calculated from the relaxation data, were used to discuss mechanisms controlling the plastic deformation rate of the UFG Cu-OF in the studied temperature range.

The temperature has a strong effect on ductility and strength of UFG copper. At room temperature the instability as a necking arises immediately after the yield stress, in contrast to temperature of 77 K where the small stage of linear hardening is observed. The absence of hardening at elevated temperatures can indicate that during plastic deformation the dynamic recovery process is dominant ones. Since the recovery is a diffusive process, at the low temperature the influence of recovery decreases so the dominant process is a hardening due to accumulation of dislocations. The thermal activation analysis has shown that at temperatures below ~ 200 K, the experimental dependences of the flow stress and the activation volume on temperature correspond to the mechanism of the thermally activated intersection of forest dislocations. Above ~ 200 K, the activation volume decreases with increasing temperature, which contradicts the mechanism of forest dislocation crossing. One of the reasons that explains this contradiction is the dynamic recovery. So for correct estimates of activation volume, it is necessary to take into account not only hardening processes, but the recovery process too. The enhancement of the role of the recovery, stimulated by the high density of dislocations in the UFG copper, leads to a significant underestimation of the activation volume, calculated from the stress relaxation data at room temperature.

Reference

- [1] V. A. Beloshenko, V. N. Varyukhin, V. Z. Spuskanyuk. Theory and Practice of Hydroextrusion, 2007, Kyiv, Naukova Dumka, 246 pp.

POSSIBLE REGISTRATION OF MAGNETIC PARTICLES IN BIOLOGICAL OBJECTS

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At present, magnetic particles (MPs) and their systems are being actively investigated for their application in biological research and medical practice. Usually magnetic particles are spheres of iron oxides (magnetite or hematite), the surfaces of which are coated with different substances. Often they are in the form of superparamagnetic particles ranging in size from 400 to 600 nm, are used to extract DNA and RNA from biological materials and in a new method of magnetic partial imaging (MPI). It is similar to magnetic resonance imaging (MRI). However, in the MPI technique, the useful signal comes directly from magnetic particles. This requires a magnetic field of several mT, while the MRI technique uses magnetic fields of several T.

In particular, we investigated composite nanomaterials consisting of bovine serum albumin (BSA) and carbon nanotubes (CNT). As usual, carbon nanotubes contain catalytic magnetic particles. Consequently, the spatial distribution of such nanomaterials can be noninvasively monitored by detecting the distribution of carbon nanotubes with the magnetic particles contained therein. Note that the BSA/CNT nanocomposite characterized by the sufficiently high strength and biocompatibility has a great potential for creating different implants, including bone or cartilage tissue substitutes [1]. We estimated the distance between a magnetic field sensor (MFS) and MP, at which the magnetic field perturbations caused by MP could be detected at different values of other parameters. It was established that magnetite particles with a specific magnetization of $50 \text{ A} \cdot \text{m}^2 / \text{kg}$, concentration 10^{12} m^{-3} and an average diameter of 50 nm can be detected by SQUIQS or combined MFS at distances of $\leq 0.1 \text{ m}$. It was mentioned that superparamagnetic iron particles and CNT containing catalytic iron particles can only be detected by SQUIDS or nanostructured combined MFS with resolution of $\sim 1 \text{ fT}$ [2].

Thus, the high-sensitivity magnetic field sensors with a resolution of $\leq 10^{-11} \text{ T}$ make it possible to detect magnetic particles in biological objects and can be used for noninvasive control of organs, implants, prostheses, and other elements in biological objects.

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References

- [1] L. P. Ichkitidze, S.V. Selishchev, A. Yu. Gerasimenko, V. M. Podgaetsky. Mechanical properties of bulk nanocomposite biomaterial. *Biomed. Eng.*, 2016, 49, 5, 308-311.
- [2] L. P. Ichkitidze, N. A. Bazaev, D. V. Telyshev, R. Y. Preobrazhensky, M. L. Gavrushina. Magnetic field sensors in medical diagnostics. *Biomed. Eng.*, 2015, 4, 6, 305-309.

EFFECT OF LASER RADIATION ON ELECTRICAL CONDUCTIVITY OF LAYERS OF BIOCOMPOSITE NANOMATERIAL

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We present the data on the electrical specific conductivity σ of the films based on biocomposite material collagen (CG) as a template filled with multi-walled carbon nanotubes (MWCNTs) deposited onto different substrates. These films are as buckypaper, but contain a small amount of carbon nanotubes (~ 0.1 wt. % of MWCNT). The conductivity of the nanomaterial films CG/MWCNT is changed (enhanced) by laser radiation.

We used CMC in the form of the aqueous solution (~ 2 wt. % CG). The water dispersion with 1 wt.% CG and a MWCNT concentration of $\sim (0.1)$ wt.% was deposited onto the substrates by screen printing. The flexible (Petri dish, polyimide, cotton fabric, and shop paper ($80 \text{ g} / \text{m}^2$)) substrates were used. Two films $(0.0005\text{--}0.02) \times 30 \times 10 \text{ mm}^3$ in size deposited onto the substrate were separated by the $\sim 0.2 \text{ mm}$ spacing. After deposition, when the films were still wet ("wet" state), one layer was coated with a lightproof layer and the other film was exposed to the continuous laser radiation with a power density of $P_s \approx 0.1 \text{ W} / \text{cm}^2$ and a wavelength of 970 nm for 20 s. The electrical properties of the films were examined after drying the samples. The conductivity of the samples was measured by four-probe methods.

The main result obtained by us is that the specific conductivity of the films increased by the effect of laser radiation. We calculated the stimulation coefficient as: $C_s = (\sigma_L - \sigma) / \sigma$, where σ is the specific conductivity of the unirradiated samples and σ_L is the specific conductivity after laser irradiation. The laser stimulation improves the specific conductivity of the films in the "liquid" state. These changes were observed in all the samples on different substrates; the σ variation for the samples deposited on to hard substrates was $C_s \sim 70 - 600 \%$. The average of C_s values for each sample was determined by measuring 4 films. The specific conductivity of the nanomaterial layers CG/MWCNT stimulated by laser radiation was approximately $0.1 - 1 \text{ kS} / \text{m}$. In addition, these films have good adhesion to soft substrates and are stable against mechanical factors. They are promising for different applications, including production of membranes for nanosized particles and materials for flexible electronics, protection of electronic circuits and biological objects from the electromagnetic radiation, fabrication of elastomers and voltage-sensing devices, and growth of biological tissues (nerve cells, muscles, etc.).

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LAYERS OF BIOCOMPOSITE NANOMATERIALS AS TENSORESISTOR

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In medical practice, it is often necessary to control motion of various body parts (e.g., joints and chest), edema, tumors, emotions, bone tissue deformation during the post-procedure recovery, etc.

For this purpose, it is convenient to use strain sensors, i.e., traditional tensoresistor gages based on metal or semiconductor materials. The tensoresistor sensors in the form of a meander made of metal foil have the low temperature resistance coefficient ($\alpha \leq 10^{-5} \text{ K}^{-1}$) and wide relative strain range ($\varepsilon = \pm 5 \%$), but low strain sensitivity ($S \leq 10$), while semiconductor tensoresistor sensors exhibit the high temperature resistance coefficient ($\alpha \geq 10^{-3} \text{ K}^{-1}$), very low relative strain ($\varepsilon \leq 0.2 \%$), and high strain sensitivity ($S \sim 100 - 200$). The tensoresistors of both types are difficult to bend and, therefore, limit motion of a biological object.

Obviously, the efficiency of a tensoresistor can be enhanced via increasing the S and ε values and decreasing the α value. However, in traditional tensoresistors it is impossible. In view of this, we studied the temperature and mechanical properties of the layers of different biocomposites nanomaterials containing single-walled carbon nanotubes (SWCNTs) in terms of their possible use as prototype of tensoresistors

The nanomaterials were prepared using different matrices (collagen (CG), bovine serum albumin (BSA), or microcrystal cellulose (MCC)) filled with SWCNTs. The matrix and filler were diluted in distilled water to obtain water dispersions of groups CG/SWCNT, BSA/SWCNT, and MCC/SWCNT with an SWCNT concentration of 0.3 wt. %.

The dispersions were used to deposit the layers by silk screening onto polyester, cotton, and office paper substrates. The resistive strain sensor prototypes were layers with a length of 15 – 20 mm, a width of 8 – 10 mm, and a thickness of 0.5 – 5 μm . Strain studies were carried out on an automated facility, which allowed controlling the tensoresistor bending angle θ , resistance, temperature, and number of measuring cycles. The bending angle varied within $\pm 160^\circ$ with a pitch of 2° . At $\theta = 0$, the resistive tensoresistor was in the initial (unstrained) position.

The dependences of resistance R on angle θ were similar for all layers: when the resistive tensoresistor was bent so as to the layers on the substrate approached one another, the resistance decreased; when the layers moved apart one another, the R value increased. At angles of $\pm 30^\circ$, the $R(\theta)$ curves represented approximately linear dependences (with an error of $\leq 10\%$); beyond this range, the dependences became nonlinear. Using the minimum bending radius ($\sim 5 \text{ mm}$) and $d \leq 1 \mu\text{m}$, we obtained the estimate $S \sim 100 - 500$, which is of the same order of magnitude as the available data or exceeds them.

The smallest value, $\alpha \sim (1 - 4) \cdot 10^{-4} \text{ K}^{-1}$, was obtained for groups BSA/SWCNT; the highest stability of the S value against moist medium was obtained for group CG/SWCNT. The high strain sensitivity ($S \sim 500$) was detected for group CG/SWCNT.

Thus, the investigated biocomposite layers prototypes as tensoresistors of groups CG/SWCNT, BSA/SWCNT and MCC/SWCNT are promising for use as strain and pressure sensors. In particular, the proposed layers as deformation sensors will be in demand for controlling the operation of an artificial muscle mounted on the surface of the heart.

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IRON CARBONATE SYNTHESIS METHOD AIMED AT OBTAINING ANTIANEMIC PREPARATION

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The medical and preventive preparation against metal-deficient (physiological) anemia, which is wide-spread in the pig breeding branch, in particular, among newborn pigs, is synthesized. The preparation contains a vital chelate complex of microelements Fe(II), Zn(II), Cu(II), Mn(II), and Co(II) with hemostimulating monosaccharide D-fructose; bioactive organic compounds – glycine, selenomethionine, and ecologically safe bentonite – Askana clay that has curative properties for gastrointestinal tract. The preparation contains the components in the following ratio (wt. %): Fe(II) – 7.5 – 9.0; D-fructose – 24.19 – 29.0; Cu(II) – 0.1; Zn(II) – 0.1; Mn(II) – 0.06; Co(II) – 0.07; glycine – 0.5; selenomethionine – 0.0000642; natural Askana clay – 68.2 – 70.9. The Fe(II) content in Fe(II)-fructose complex obtained as a result of interaction of the main antianemic microelement – iron source $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$ and D-fructose is 74.34 %, while 25.66 % are in oxidized Fe(III) condition [1]. Preparations with relatively low bioassimilation in the targeted product, manufactured on the basis of high content of trivalent iron ions, are characterized by insufficient efficiency [2].

There is elaborated the method, which foresees the use of newly-prepared FeCO_3 as the iron source. FeCO_3 is obtained through the interaction of hot saturated solutions of NaHCO_3 and $\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$, under constant stirring conditions. The reaction runs with gas (CO_2) emission. The precipitate formed after precipitation is dewatered using decantation. Afterwards the precipitate is washed thoroughly first in the flowing water, then in the distilled water till the complete removal of chlorine ions.

Green-colored iron(II) carbonate is obtained, which is kept under water layer (in order to prevent bivalent iron ions from oxidizing into trivalent ones). Iron-fructose complex synthesized by the mentioned way contains bivalent iron in quantities foreseen by the assigned task. As a result, the targeted product – medical and preventive antianemic preparation with high content of Fe(II) ions having high bioaccessibility is obtained that secures therapeutic and preventive efficiency of the medication.

Preparation assimilation is also improved by the processing of the system containing Askana clay and the rest components using the ultrasound dispergation method (under conditions of 22 kHz), through preparation particles' dispergation down to nanosizes that is considered as a new, prospective direction of nanomedicine [3]. Rheological properties of the preparation with hydrophilic properties manufactured using newly-prepared iron carbonate have been studied with the rotation viscometer "Reotest 2", in the gastric juice acidity range characteristic for suckling pigs and young pigs, which equals to $\text{pH} = 3.5 - 4.0$ and $2.5 - 3.0$, respectively.

As is seen from the **Table 1**, according to rheological and structure-forming parameters the preparation meets all requirements imposed to therapeutic agents.

Table 1. Rheological characteristics of 8 %
water suspension of antianemic preparation.

Research subject	pH	Plastic viscosity		Conventional yield limit		Static plasticity
		Initial η , Pa · s	Smallest η , Pa · s	Static Pk_1 , Pa	Dynamic Pk_2 , Pa	Pk_1 / η_1 , $10^{-2} s^{-1}$
Askana clay	3.5	490	8.80	0.96	2.60	19.50
	2.0	1700	3.30	2.40	2.72	14.10
Antianemic preparation	3.5	22	0.43	0.30	0.75	1.30
	2.0	161	1.41	2.00	3.75	1.24

References

- [1] Ts. Gabelia, L. Japaridze, E. Salukvadze, L. Kashia, S. Urotadze. Determination of Fe(II)/Fe(III) ions' ratio in iron-fructose complex. Herald Georg. Natl Acad. Sci. (Chem. Ser.), 2009, 35, 1, 36-39.
- [2] N. N. Stuklov, E. N. Semyonova. Treatment of irondeficient anemia. What is more important: Efficiency or tolerance? J. Int. Med., 2013, 1, 2, 47-55.
- [3] O. A. Gromova, I. V. Gogoleva. Selenium – impressive results and application prospects. Medicine of Emergency, 2010, 6, 31, 37-52.

NEGATIVE PHOTOELECTRIC EFFECTS RESEARCH BY USE OF EQUIPMENT “POLYCHROMATOR”

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Nowadays, there is a growing interest in the optical properties of heterostructures with nanoscale clusters, quantum wells and quantum dots based on Si, SiGe, $A^{III}B^V$, and $A^{II}B^{VI}$ semiconductor materials, etc. The main goal is to fabricate photosensors based on these materials for different optical ranges. Of particular interest was a negative photoelectric effect observed in these structures. When measuring the photoconductivity of the detectors on a monochromator to reveal this effect, the researchers had to resort to additional illumination of the samples in order to change the charge state of the trapping centers of charge carriers. This complicates both carrying out of the experiment and interpretation of the results obtained.

In our experiments, under real conditions, the photosensitive element is exposed to a beam of light of a limited wavelength range rather than to a non-monochromatic light, we developed a genuine technique and created a setup called “Polychromator”, enabling illumination of samples with “packets” of non-monochromatic light [1 – 8]. In the development of microelectronic technologies, along with other methods of investigation of physical properties of semiconductor materials and devices created thereon, optical methods are also very important. These methods are invaluable for investigation of physical properties of optoelectronic devices and various types of electromagnetic radiation sensors. Optical methods of measurement have proved particularly effective and efficient in terms of occurrence of nanotechnological materials, since they do not require a strong impact on the material and do not entail its structural (even local) destruction, which attracts great attention to these new methods. We have created a setup “Polychromator” – a new device for studying optical properties of semiconductor materials and structures. In this setup, by sequentially changing optical filters in the optical range of 200 – 4100 nm we single out electromagnetic radiation packets and study the photosensitivity of the structures under investigation, such as photosensors, not only at one wavelength, but within the whole spectral packet.

It appeared that in a number of spectral ranges, spectral photosensitivities taken both by a monochromator and a polychromator differ essentially. In our opinion, the proposed setup and methods of research open up new possibilities for the study of physical properties of materials, structures and devices of modern electronics created on their basis.

References

- [1] N. Khuchua, M. Tigishvili, N. Dolidze, Z. Jibuti, R. Melkadze, R. Diehl. Ch. 7: Ion Implantation as a tool for controlled modification of photoelectrical properties of silicon. In: Ion Beam, Applications (Ed. I. Ahmad), 2018, IntechOpen, 139-159, DOI: 10.5772/intechopen.76992.

- [2] L. Jibuti, Z. Jibuti, R. Melkadze. The original method for studying optical properties of semiconductor materials and structures and the setup “Polychromator”. In: Abs. 4th Int. Conf. “Nanotechnologies”, 2016, Tbilisi, GTU, 89-89.
- [3] M. Tigishvili, N. Gapishvili, R. Gulyaev, Z. Jibuti, N. Dolidze, N. Khuchua, R. Melkadze. Mint: Defect engineering in the silicon p-n junction technology. Geor. Eng. News, 2013, 68, 75-79.
- [4] N. Khuchua, N. Dolidze, N. Gapishvili, R. Gulyaev, Z. Jibuti, R. Melkadze, M. Tigishvili. Mint: Technology of semiconductor materials sensitive to different regions of the electromagnetic radiation spectrum. Nanotechnology Perceptions, 2014, 4, 91-99.
- [5] M. Tigishvili, N. Khuchua, R. Melkadze, N. Dolidze, G. Gapishvili, Z. Jibuti, G. Dovbeshko, V. Romanyuk. Semiconductor material with new optical properties for infrared and ultraviolet photodetectors. In: Proc. 2nd Int. Conf. “Mod. Technol. & Meth. Inorg. Mater. Sci.”, 2015, Tbilisi, Georg. Natl. Acad. Sci. Press, 288-295
- [6] N. Dolidze, Z. Jibuti, M. Tigishvili, N. Khuchua, R. Melkadze, N. Gapishvili. Effect of light spectral composition on photoelectric properties of ion doped silicon. In: Proc. Int. Conf. “Adv. Mater. & Technol.”, 2015, Tbilisi, Georg. Natl. Acad. Sci. Press, 63-67.
- [7] N. Khuchua, M. Tigishvili, R. Melkadze, N. Dolidze, N. Gapishvili, Z. Jibuti, G. Dovbeshko, V. Romanyuk. Defect formation in ion-implanted Si – Approach to controlled semiconductor optical properties. Solid State Phenomena, 2016, 242, 374-379.
- [8] M. Tigishvili, N. Khuchua, N. Gapishvili, T. Sakharova, N. Dolidze, Z. Jibuti, G. Peradze, R. Melkadze. Impact of damages in monocrystalline n-Si on material photosensitivity. Physica Status Solidi C, 2017, 14, 1700094, 1-6.

SYNTHESIS OF NITRIDE NANOMATERIALS IN PRESENCE OF HYDRAZINE AND AMMONIUM CHLORIDE VAPOR

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The formation of crystalline nitride materials is a complicated task, which usually needs the high temperature processes and the application of active nitriding precursors. Previously, we have developed the hydrazine-based technology for producing such nitride nanomaterials as germanium and indium nitrides. The purpose of this work was to further improve this technology by adding the ammonium chloride (NH_4Cl) to hydrazine (N_2H_4), and to investigate the formation of Ge and boron nitrides using this technology.

The germanium nitride was chosen as a model material, because its formation in a poor hydrazine was studied in details, allowing for the comparative study of differences between the hydrazine-assisted and hydrazine+ammonium chloride-based processes. The interest for the growth of BN nanomaterials was caused by its unique physical properties and the ability of h-BN to form the layered 2D nanostructures.

The grown nanomaterials were characterized by scanning electron microscope (SEM), X-ray diffraction (XRD), energy dispersive spectroscopy (EDS).

The analysis of thermochemical reactions that involved the precursor existing in the reactor revealed that in the case of Ge and B sources the reactions that lead to the formation of Ge_3N_4 and BN are thermodynamically most favorable.

The nanostructures containing BN layers were synthesized on Si substrate during 20 hours at 700°C . They were also subjected to Rapid Thermal Annealing. The formation of h-BN was confirmed by XRD and EDS analysis. The thickness of BN layers was well below 100 nm. As for germanium nitride, the $\alpha\text{-Ge}_3\text{N}_4$ nanowires were synthesized on Ge substrate at 440°C . This synthetic temperature is by 60 and 410°C lower than the growth temperature of the same material using hydrazine or ammonia.

The obtained results clearly demonstrated that in the vapor of a mixture of $\text{NH}_4\text{Cl} + \text{N}_2\text{H}_4$ the active nitriding precursors are formed, which enable the low temperature growth of nitride nanomaterials.

PERFORMANCE OF BORON NITRIDE COATINGS ON CUTTING TOOLS AND DIES

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Boron Nitride (BN) coatings are applied on cutting tools and dies to increase their working lives, to decrease their wear and contact friction and to increase their hardness. BN has several allotropes (polymorphs). They are: hexagonal (h-BN), cubic (c-BN), rhombic (r-BN), wurtzite (w-BN), amorphous (a-BN), turbostratic (t-BN), and explosive (e-BN).

While h-BN is soft and lubricious, c-BN is the hardest material after diamond. The other allotropes have properties in between these two extremes. BN is a good conductor of heat but does not conduct electricity. It has a very high melting point as 2953 °C. These properties also increase the effectiveness of BN coatings on tools and dies. BN coatings are applied on cutting tools and dies by using a PVD system enhanced by magnetron sputtering and microwave (**Figures 1 and 2**).



Figure 1. PVD coating system.



Figure 2. Coated tools.

Substrates are mainly hardened tool steel and carbide. Their surfaces are cleaned mechanically and by ultrasonic methods to remove any oxides. Also after chemical cleaning they are placed in the vacuum chamber of the PVD coating system. After final cleaning by resputtering of the substrate by RF energy, BN coating starts by using RF energy on the magnetron where magnetic sputtering is also applied. Using Ar and O₂ gases in the plasma environment, at high vacuum, BN coating continues for specified hours.

The coated tools are then removed and surface characterizations of the coating are done. This includes the nano hardness, scratch, thickness, tribometer and FTIR tests. Surface characterization results can be affected by coating parameters.

The samples are then tested in the real environment in the industry either in cutting or forming [1 – 3]. It is seen that, generally, the life of the tool is increased up to about four times. The decrease in surface friction during cutting also improves the surface finish of the workpiece.

References

- [1] T. Ozel, T. Thepsonthi, D. Ulutan, B. Kaftanoglu. Experiments and finite element simulations on micro-milling of Ti–6Al–4V alloy with uncoated and cBN coated tools. CIRP Ann. Manuf. Technol., 2011, 60, 85.
- [2] B. Kaftanoglu, N. Dokmetaş. Performance of boron nitride coated tools and dies. In: Adv. Prod. Eng. & Manag., 8, 2013, Prod. Eng. Inst., 177.
- [3] B. Cetin, G. Durkaya, H. Kurtuldu, T. Hacaloglu, M. Gurbuz, B. Kaftanoglu. Wear resistance performance of boron nitride coatings on end milling cutters. Int. J. Mechatron. & Manuf. Syst., 2017, 10, 3.

**STUDY OF DISTRIBUTION OF NATURAL RADIONUCLIDES
IN SOILS AND ASSESSMENT OF EXPOSURE
HAZARDS FROM TERRESTRIAL GAMMA RADIATION
ON EXAMPLE OF TSALKA REGION (GEORGIA)**

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Natural radioactive substances in the soil are constant sources of human radiation hazards. The average annual dose rate coming from natural sources equals to 2.4 mSv, whereas the share of radiation from artificial sources is 0.8 mSv / y [1]. Thus, 75 % of total radiation affecting human health falls on natural radiation sources. Consequently, the great importance of studying the existing natural radiation of radioactive sources and assessment of threats caused by radiation hazard is quite apparent. 19 soil samples were collected from Tsalka region (South Georgia). Gamma-spectroscopy method was used to determine the activity concentrations (in Bq / kg) of natural radionuclides of ²³⁸U, ²³²Th and ⁴⁰K in soil samples. Based on results, it was calculated contents of radionuclides in soil (in g / kg and in ppm). Besides, there was determined the concentration of artificial radionuclide ¹³⁷Cs in soil samples, which gave us opportunity to assess the contamination character of the area under study. Based on the results, was calculated some crucial physical values necessary to assess the radiation exposure hazards of the population. Particularly, there was determined the absorbed gamma dose rate in the air; Annual effective dose rate; External hazard index and Radium equivalent activity which is used in the assessment of radioactive industrial materials. Obtained results were compared with a results given in similar works carried out in other countries, as well as with mean values (results) and recommendations given by international organizations (UNSCEAR and ICRP).

Reference

- [1] United Nations Scientific Committee on the Effects of Atomic Radiation. Report of UNSCEAR to the General Assembly, United Nations, 2000, New York, UNSCEAR.

INFLUENCE OF DISPERSION MEDIUM ON PROPERTIES OF CdTe MICRO- AND NANOCRYSTALS IN COLLOIDAL SOLUTION

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The influence of commonly used dispersion media on the formation of micro- and nanocrystals CdTe stabilized by thioglycolic acid (TGA) was investigated. Surface and optical properties of CdTe nanoparticles obtained by grinding (40 – 150 nm, microcrystals) and colloidal synthesis (1 – 4 nm, nanocrystals) methods were investigated. It was shown that the most intense adsorption of stabilizer molecules on the CdTe surface occurs with solvents which are better wetting the surface of CdTe particles. The best stabilization of both the micro- and nanocrystals of CdTe occurs, when methyl and ethyl alcohol is used as the dispersion medium.

The basic characteristics of photoluminescence of CdTe nanocrystals stabilized with thioglycolic acid (TGA) in deionized water, methanol and ethanol of various concentrations were investigated. It has been shown that introduction of finely grinded CdTe nanocrystals into inorganic (water) and organic (methanol, ethanol) solvent results in their different surface properties, reflected in a different adsorption intensity of TGA molecules. This is supposed to be determined by the nature of the interaction between stabilizer and adsorbent (CdTe) and by adhesive energy in the system solvent-CdTe. It has been found that the adsorption isotherms of CdTe nanocrystals in water, methanol and ethanol are *S*-shaped. The intensity of adsorption of the stabilizing molecules (TGA) was found to be proportional to the wettability of the CdTe surface with the corresponding solvent. It was demonstrated that the nature of the dispersion medium influences also drastically on optical properties synthesized NCs in this medium by a colloidal (bottom-up) approach. In particular, adding monoatomic alcohols to the aqueous reacting solution increases the stability of the resulting colloid to sedimentation and eliminates the defect-related photoluminescence emission. However, the intensity of the excitonic emission in the alcohol-containing samples is partially reduced compared to purely water solutions.

ELECTRICAL PROPERTIES OF PEDOT:PSS/CNTS NANOCOMPOSITES AT LOW TEMPERATURES

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One can define carbon nanotubes as cylindrical objects that are formed as the result of envelopment of the graphene layer. Carbon nanotubes, or CNT, are cylindrical objects with a high aspect ratio that results from wrapping a graphene layer onto itself. In case there is a single graphene layer, the structures obtained are referenced to as single-walled carbon nanotubes (SWNTs). If a few layers of graphene are wrapped, the resulting formations are called multi-walled carbon nanotubes (MWNTs). The behavior of electrical properties of PEDOT:PSS/CNT composites as a function of frequency was also studied recently [1]. In this work systematic study of electrical properties of PEDOT–PSS polymer composites reinforced with single-walled and multi-walled carbon nanotubes on the temperature range of 50 – 200 K were performed.

Hybrid composite films were prepared starting from 1% water suspension of poly-3,4-ethyldioxiophen. Two types of nanofiller were used: purified (90 wt. %) single-walled carbon nanotubes (SWCNTs) with average diameter of 1 nm and purified multiwalled carbon nanotubes (95 wt. %) with average outside diameter of 65 nm, average inside diameter of 10 nm (MWCNTs).

Prepared samples of PEDOT:PSS/CNTs composite films were subjected to low-temperature impedance measurements. Temperature dependencies of the measured sheet resistance of the SWCNT and MWCNT reinforced composite films were measured at 100 kHz frequency in the range of 50 to 200 K. Reasons for selecting such temperature range limits were (i) relatively small variation of resistance from 200 K up room temperature (total resistance at higher temperatures is determined by random network of nanotubes with tunneling barriers between individual tubes i) and (ii) rapid increase of resistance for SCWNT composites below 50 K, so that the values of R were beyond the range of measurements for RLC meter.

Generally, lateral resistance of PEDOT:PSS/CNTs composite films increases non-linearly upon cooling. The dependencies are split in two sub-ranges, since, as shown below, there are possibly different mechanisms involved below and above 90 K. As far as different loadings of nanofiller are considered, sheet resistances decrease with nanotube concentration.

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Reference

- [1] A. Benchirouf et al. *Sensors and Actuators B*, 2016, 224, 344-350.

DOSE-DEPENDENT STRATEGIES OF BIOCHEMICAL
ADAPTATION OF *Fagopyrum Esculentum* PLANTS
UNDER ALUMINA NANOSCALES TREATMENTS

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Aluminum (Al) is most widespread element in the lithosphere. Toxicity of its ions has noticeably negative effects on growth and development of plants species growing on acid soils. Al influence manifests as limitation of the productivity of crop plants by 30 – 40 %. At the same time, it was observed that Al applied at low concentrations can stimulate plant growth. Nowadays the Buckwheat genus (*Fagopyrum* Mill.) is one of the most studied Al resistant crops due to Al-hyperaccumulating capability.

Colloidal solution of Al-based nanoscales was received by electric-sparkle dispersing of electric-conductive layer in the water. Specimens of the X-ray analysis were conducted by using aUltima IV (Rigaku) diffractometer with monochromatic Cu $K\alpha$ radiation. For investigation were used 21 day controlled and treatment plants of common buckwheat (*Fagopyrum esculentum* Moench. cv. Rubra). In the experiment were used the following concentrations of Al nanoscales: 50, 250, 500, 750, and 1000 mg / L.

X-ray analysis showed three phase components in the polycrystalline specimens – Al(OH)₃ with monoclonal structure (39 nm), Al₂O₃ gamma oxide with tetragonal structure and polymorphic modification of Al(OH)₃ with triclinic structure (11 nm). Enhancement effects of Al-based nanoscales on all pigments classes were noted in variants with 50 and 250 mg / L. Chlorophyll b and carotenoids increasing were observed in variants with 500 and 750 mg / L of Al-based nanoscales. Total soluble protein content increased in variants with 50, 250, and 500 mg / L, but decreased in variants with 750 and 1000 mg / L of Al nanoscales. The results of the study of the effects of Al nanoscales on phenolic and anthocyanin contents showed that addition of nanoscales induced the anthocyanin accumulation with a dose-dependent relation. Addition of 1000 mg / L of Al-based nanoscales led to maximum stimulatory response – 241% of control level. The sharp increase of total phenolic content fixed in all variants of Al-based nanoscales treatments.

Thus, the presence of Al (Al(OH)₃/Al₂O₃) nanoscales in low concentrations (50 and 250 mg / L) induced total soluble protein synthesis, phenolic compounds and anthocyanin accumulation, led to increasing of chlorophylls and carotenoids content.

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PRODUCING OF InGaAs BULK CRYSTALS BY DIRECT FUSION

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The system of continuous solid solutions of III–V binary compounds $\text{In}_{1-x}\text{Ga}_x\text{As}$ allows solution of many problems of modern semiconductor technology as microelectronics, optoelectronics, and nanotechnology. The remarkable manufactural properties of $\text{In}_{1-x}\text{Ga}_x\text{As}$ ternary solid solutions make them truly revolutionary nanotech performance materials and very useful for manufacture nanotech products, such as nanowires, nanotubes, etc. For successful solution of this problem, it is necessary to reveal their intrinsic properties and eliminate the effect of structural imperfections existing in thin films and layers, which is possible by investigating crystals of $\text{In}_{1-x}\text{Ga}_x\text{As}$ solid solutions in bulk form. Much effort has been focused on $\text{In}_{1-x}\text{Ga}_x\text{As}$ technology intended for different purposes and scales of application, which has been realized by using many known traditional methods. In given work direct fusion process of InAs GaAs components and the crystal growth method of their solid solutions is used for producing $\text{In}_{1-x}\text{Ga}_x\text{As}$ solid solutions. At choice of producing method it has been taken into account the complete miscibility of components in the solid state and the linear dependence of lattice parameter on the composition of $\text{In}_{1-x}\text{Ga}_x\text{As}$ solid solutions. These properties allow to consider this system as a pseudo-binary alloys system of two components of $(\text{GaAs})_x$ and $(\text{InAs})_{1-x}$ like SiGe system. The proposed method is fundamentally different from the methods for obtaining $\text{In}_{1-x}\text{Ga}_x\text{As}$ crystals with a certain composition in one ingot, and, in turn, requires other conditions of the processing of crystal growth. Carefully selected conditions of fusion allowed of obtaining uniform in composition of components across the ingot several compositions of InAs-rich InGaAs solid solutions with one fusion.

STOCHASTIC FILTRATION METHOD SIMULATION OF PROCESSES DETECTION AND STANDING OUT CANCER CELLS BY MACROPHAGES WITH EMBEDDED FE NANOPARTICLES

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The use of inorganic nanoparticles, in particular metals, opens up broad prospects in biology and medicine. Thus, the biological activity of copper nanoparticles provides highly effective treatment of purulent wounds tissue healing [1, 2]. At the same time, nanoparticles generated by electrophysical technologies are most preferable, since they have the greatest value of free energy [3, 4]. This fact must be taken into account when developing technologies for generating nanoparticles.

The field of application of metal nanoparticles in the diagnosis and therapy of malignant tumors is actively developing. In [5], on the example of metallic gold nanoparticles, the prospects of developing a method for local thermal damage of tumor cells due to laser heating of nanoparticles at the wavelength of plasma resonance are considered. The accumulation of nanoparticles in macrophages littoral dendritic cells of the iliac lymph node and in hepatocytes is shown.

As it is shown in [6], the absorption of iron nanoparticles gives macrophages the ability to detect and inhibit cancer cells that previously remained invisible. This ability of macrophages, acquired as a result of the absorption of iron nanoparticles, can be modeled in the radar problem of target detection and isolation against the background of the presence of numerous objects that create a complex radar situation that can be represented as a model of high-intensity white Gaussian noise.

The solution of the problem of the signal standing out from the mixture of the background high-intensity Gaussian noise can be provided by the method of nonlinear filtering based on the stochastic resonance effect [7, 8]. The main advantage of the method is the use of noise as an energy source, which, as a result of nonlinear conversion in a stochastic filter, provides an increase of the signal-to-noise ratio at the output of the filter.

A model based on a stochastic nonlinear filter is proposed for describing the process of standing out of cancer cells by macrophages that have absorbed iron nanoparticles. A mathematical model of the filter is developed and the results of calculations for the harmonic signal model and the pulse signal on the background of intensive white Gaussian noise are presented.

References

- [1] I. V. Babushkina. Metal nanoparticles in the treatment of experimental purulent wounds. *Saratov Sci. Med. J.*, 2011, 7, 2, 530-533.

- [2] S. I. Gulchenko, A. A. Gusev, O. V. Zakharova. Perspectives of creation of antibacterial preparations based on copper nanoparticles. *Tambov Univ. Herald (Ser. Nat. & Tech. Sci.)*, 2014, 5, 19, 1397-1399.
- [3] Yu. A. Kotov. Electric explosion of wires as a method for preparation of nanopowders. *J. Nanopart.*, 2003, 5, 539-550.
- [4] V. Chumakov, O. Stolarchuk, M. Ostrizhnoi. Electrical exploding wires as the source of nanoparticles. *Am. J. Nanosci.*, 2016, 2, 4, 51-55.
- [5] Yu. P. Meshalkin, N. P. Bgatova. Prospects and problems of using inorganic nanoparticles in oncology (Review). *J. Siberian Federal Univ. (Ser. Biol.)*, 2008, 1, 3, 248-268.
- [6] A. Tarangelo, S. J. Dixon. Nanomedicine: An iron age for cancer therapy. *Nat. Nanotechnol.*, 2016, 11, 921-922.
- [7] O. I. Kharchenko, A. M. Gorban. Non-linear filtering of pulse signals in case of high intensity noise. *Prob. At. Sci. & Technol. (Ser. Nucl. Phys. Investig.)*, 2017, 6 (112), 113-116.
- [8] O. I. Kharchenko, V. M. Kartashov. Digital signal extraction by means of nonlinear stochastic filtration. *Bull. Natl. Tech. Univ. Ukr. "KPI" (Ser. Radio Tech. & Radio Apparatus)*, 2018 – *in press*.

SOLUBILIZATION AND DISPERSION OF CARBON NANOTUBES AND OTHER CARBON ALLOTROPES

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The carbon nanotubes (CNTs), one of the best novel nanostructures and classic objects in nanotechnology, form bundle-like structures with very complex morphologies with a high number of van der Waals interactions, causing extremely poor solubility in water or organic solvents. Due to their exceptional combination of mechanical, thermal, chemical, and electronic properties, single-walled (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) are considered as unique materials, with very promising future applications, especially in the field of nanotechnology, nanoelectronics, and composite materials. Additionally, CNTs are becoming highly attractive molecules for applications in medicinal chemistry. At present, potential biological and medical applications of CNTs have been little explored, in particular for drug delivery purposes. The main difficulty to integrate such materials into biological systems derives from their lack of solubility in physiological solutions. Functionalization of CNTs with the assistance of biological molecules remarkably improves the solubility of nanotubes in aqueous or organic environment and, thus, facilitates the development of novel biotechnology, biomedicine and bioengineering. Many of these applications require an increased “solubility” of CNTs in solvents [1], first of all in water, especially for biological applications. This could be reached by their functionalization, which is a very actively discussed topic in contemporary literature because the planned modification of CNTs properties is believed to open the road towards real nanotechnology applications. It is difficult to prepare an aqueous dispersion of CNTs stable for months; their insolubility has been a limitation for the practical applications of this unique material. Proper dispersion of CNTs materials is important to retaining the electronic properties of nanotubes. The redissoluble functional compound/CNTs composites are needed for post processing, because CNTs dispersions usually easy aggregate and, therefore, to become additional processing very difficult.

Available solubilization methods

A series of contemporary techniques are being used for CNTs solubilization, from *physical* (classic ultrasound, plasma treatment or UV-light) to *chemical* and *biological*, applying inorganic (other carbon allotropes, iodine, metallic sodium in liquid ammonia, CO₂, peroxides, metal salts and mineral acids) and organic (acids, salts, polymers, dyes, natural products and biomolecules) compounds, as well as micelles on their basis and some metal complexes. Frequently, physical action (more frequently ultrasound, more rarely hydrothermal technique) is combined with chemical/biological treatment. In some cases, successive steps can be applied, for instance use of low- and high-weight surfactants, mineral acid treatment for creation of –OH and –COOH groups and their further interaction with organic molecules. Carbon nanotube dispersion in nematic liquid crystals is also known.

Important observations and considerations

It has been suggested that van der Waals interaction, π - π stacking interactions between aromatic rings in organic compounds and CNTs, and hydrophobic interaction are major factors

that are responsible for the CNTs dispersion. Choosing *surfactants*, to be able to stabilize carbon nanotubes in water, it is necessary to employ such dispersing agents that a) strongly adsorb on the nanotube surface, b) present hydrophilic groups, better if rigid, that extend toward the aqueous phase, c) are not very mobile on the nanotube surface, and d) show aggregates with structure dependent on nanotube diameter and chirality.

For appropriate *solvent selection*, it was established for SWCNTs case that 1) heavier solvents (and small in size) most probably are better solvents for SWCNTs, 2) higher polarizability of the solvent molecule increases the dispersibility. Among solvents, water is most preferable due to much more existing and potential CNTs applications, in particular more for medical and biological purposes. N-methyl-2-pyrrolidinone (NMP), N-dodecyl-pyrrolidinone (N12P), acetone, tetrahydrofuran (THF), N,N-dimethylformamide (DMF), N,N-dimethylacetamide (DMA), cyclohexyl-pyrrolidinone (CHP) have been considered as suitable solvents for CNTs dispersion, meanwhile, in contrast, much precipitation can be obviously observed for systems of the CNTs in water, ethanol and toluene.

Each discussed method leads to an improvement of CNTs “*solubility*”, frequently considerable. The formed dispersions could be stable for long periods of time, from several weeks to some months, even sometimes remained stable after centrifugation. Sometimes, unpredictable results could occur, such as, for example, in case of action of humic acid to effectively disperse MWCNTs, but not SWCNTs, into stable suspensions under the studied conditions, or when structures of amorphous carbon and carbon particles of MWCNTs were completely eliminated and the tips of nanotubes opened applying planetary ball mill.

Some curious, but naturally determined and explained observations were emphasized by researchers, in particular on better dispersibility of the CNTs with bigger diameters (treatment with plasma or graphene oxide) or more favorable suspension of CNTs using negatively charged nanodiamonds as compared to positively charged particles, possibly caused by electrostatic interactions. The presence of *π -conjugated systems* that can potentially interact with CNTs to induce its dispersion is considered as a contributing factor, as well as both hydrophilic and hydrophobic moieties in amphiphilic bifunctional molecules. Additionally, a huge number of *polyaromatic compounds* (especially pyrene derivatives) and a variety of polymers and biomolecules are noted to be used as surfactants or functionalizing agents. As an example, bifunctional molecules with pyrene groups exhibited high CNTs solubility in common organic solvents with very different polarities such as tetrahydrofuran, toluene, and *n*-hexane. Several special studies have been carried out in the areas of influence of solvent and light on CNTs dispersibility, combinations and abilities of surfactants, CNTs cytotoxicity, etc.

In addition to CNTs, there are, although considerable lesser information, on the solubilization of other carbon allotropes and nanocarbons, for example graphite, nanoonions, fullerenes, graphene, nanodiamonds, nanodots, etc.

Reference

- [1] O. V. Kharissova, B. I. Kharisov. Solubilization and Dispersion of Carbon Nanotubes. 2017, Springer-Nature, 258 pp.

ROLE OF PHANTOM DESIGN FOR BRAIN RESEARCHES

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One of the important parts in brain research is the experiment, in this case representing cylindrical phantom measurements.

Phantom experiments are important for many reasons, for example, the brain scan is not always possible, therefore, various forms of the phantom (cylindrical, traversal, parallel, etc.) are used, which almost exactly represents brain fibres adhesion.

Its design constitutes the cylindrical shape and it is made of plastic materials. Inside it the plastic tube is also placed, being wrapped around 10 m / m filamentary fibres, which, in turn, constitutes the analogue of regions connecting fibres in the brain.

The main objective of the conducted experiments was the homogeneity of the signal, since in the case of the cylindrical phantom, the signal from fibres along the magnetic field is stronger, than from fibres, which are perpendicular to the magnetic field. It depends on the susceptibility of the magnetic field.

In this case, for fibres arranged along the magnetic field the signal is present, while for perpendicular fibres, there is a noise only and, thus, results are wrong.

The experiments were conducted in a cylindrical phantom and maximal scanning time was about 40 minutes with different numbers of parameters. During the experiment it is very important the necessity of keeping the severe safety rules.

X-RAY STRUCTURAL ANALYSIS OF SILICON

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The control of impurities at each stage of the purification process of Si is the primary topical problem in Si technology. The technique of determining the impurity composition should be multi-element and with low limit-detection of impurities. From this point of view, X-ray structural analysis of the phase composition of Si, based on the identification of X-ray diffraction lines, is very attractive. At present, the searching of new low-cost and efficiency methods of purifying Si, researchers often apply to metallurgical methods. Therefore, the investigation of obtaining of Si directly from MG-Si is attractive to reveal the physical possibilities of the directional crystallization. In given work there are considered the possibilities on a set of detectable impurities and the limits of their detection in such type of Si by X-ray diffraction method. It has been shown, that applicability of X-ray structural analysis of the phase composition of Si, based on the identification of X-ray diffraction lines, depends on the stage of Si purification.

HETEROMETALLIC CARBOXYLATE COMPLEXES AS SECONDARY BUILDING UNITS IN MOFs

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Metal organic frameworks (MOFs) are a class of crystalline materials characterized by an open framework that can be porous (porous materials). MOFs are perspective materials and can be used for gas storage, purification and separation, as well as in catalysis and sensing applications. Direct synthesis of MOF containing polynuclear metal fragments can be carried out in two ways, reaction of metal salt(s) and organic linkers or use of polynuclear molecular complexes in ligand exchange reactions. Both methods have some advantages and disadvantages and the construction of a framework of polynuclear fragments (secondary building units (SBUs [1]) opens up new prospects associated with the diversity of structures and topologies, as well as the properties of framework determined by nature of metal ions (d or $4f$) or combination of metal ions (d and $4f$) in SBU [2]. The main problem of the second approach is the choice of molecular complexes having stability of metal core structure in the ligand exchange reactions.

Combination of different metal (Li – d , $4f$) salt resulted in formation of new polynuclear heterometallic carboxylate complexes that reveal interesting luminescence and magnetic properties. The presence of carboxylate groups in the complex makes it possible to rely on the use of such compounds as precursors for the synthesis of MOFs in the ligand exchange reactions of monocarboxylate groups for dicarboxylate [3, 4]. The presented report will demonstrate a new series of molecular carboxylate complexes (Li – $3d$, $3d-3d'$, $d-4f$) with interesting individual chemical and physicochemical properties and their ability to be the precursors for SBUs in MOFs.

References

- [1] M. Eddaoudi, D. B. Moler, H. L. Li, B. L. Chen, T. M. Reineke, M. O’Keeffe, O. M. Yaghi. *Acc. Chem. Res.*, 2001, 34, 319.
- [2] D. N. Dybtsev, A. A. Sopianik, V. P. Fedin. *Mendeleev Comm.*, 2017, 27, 321.
- [3] A. A. Sopianik, E. N. Zorina–Tikhonova, M. A. Kiskin, D. G. Samsonenko, K. A. Kovalenko, A. A. Sidorov, I. L. Eremenko, D. N. Dybtsev, A. J. Blake, S. P. Argent, Martin Schroöder, V. P. Fedin. *Inorg. Chem.*, 2017, 56, 1599.
- [4] A. A. Sopianik, M. A. Kiskin, D. G. Samsonenko, A. A. Ryadun, D. N. Dybtseva, V. P. Fedin. *Polyhedron*, 2018, 145, 147.

MODELING OF AGEING PROCESSES IN FUNCTIONAL CERAMICS AND NANOSTRUCTURED THICK-FILM STRUCTURES

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The degradation kinetics are modelled at the examples of thermally-induced ageing effects in the temperature-sensitive spinel-type bulk functional ceramics based on mixed transition-metal manganites and their nanostructured thick-film structures. It was shown that degradation transformations in these materials, described by ideal exponential function, are determined exceptionally by one value of activation energy whichever the structural dispersivity of the system. In contrast, the non-exponential degradation kinetics corresponds strongly to two boundary cases, described by stretched (with power index $0 < \kappa < 1$) or suppressed (with power index $\kappa > 1$) exponential-power-low relaxation functions [1]. The stretched exponential-power-low character is proper to own degradation transformations in bulk functional ceramics independently on their phase composition and impurities. This type of ageing kinetics was considered at the example of $\text{Cu}_{0.1}\text{Ni}_{0.1}\text{Co}_{1.6}\text{Mn}_{1.2}\text{O}_4$ ceramics caused by more than 500 h annealing at 443 K. The degradation transformations are described by suppressed exponential-power-low kinetics. It was established that suppressed character is explained by two interconnected processes, the first one being the burning-off in organic binder remainders and the second one being the penetration of contact material into thick films.

The kinetics dependences of thermally-induced drift of electrical resistance in single- and multilayered temperature-sensitive thick-film structures based $\text{Cu}_{0.1}\text{Ni}_{0.1}\text{Co}_{1.6}\text{Mn}_{1.2}\text{O}_4$ (with p^+ -types of electrical conductivity), $\text{Cu}_{0.1}\text{Ni}_{0.8}\text{Co}_{0.2}\text{Mn}_{1.9}\text{O}_4$ (with p -types) ceramics are investigated also. It is established, that two interconnected processes are activated during degradation test in p - and p^+ -type thick film – the burning-out of remainders of organic binder between contacting spinel grains with simultaneous Ag penetration into appeared free-volume space. The degradation kinetics are described by the suppressed relaxation function for p - and p^+ -type thick films and extended function for p^+-p thick-film structures.

I. Karbovnyk thanks the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska–Curie Grant Agreement No 778156.

Reference

- [1] H. Klym, V. Balitska, O. Shpotyuk, I. Hadzaman. Microelectronics Reliability, 2014, 54, 12, 2843-2848.

TITANIUM NITRIDE INTERLAYER MEMRISTORS

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Memristor is two-terminal, non-volatile, non-linear element [1]. Its fingerprint is hysteresis and dominance of ionic conductivity [2, 3].

In the following presentation the technological processes of receiving and researching of memristor with different active is discussed. Memristors main active layers have been made of titanium dioxide with different stexiometries of TiO_{2-x} (Figure 1).

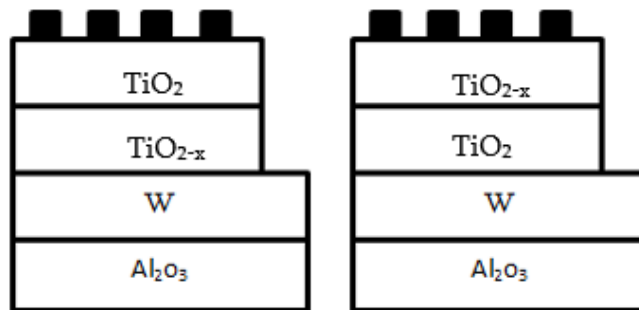


Figure 1. Memristors different configurations with TiO_2 and TiO_{2-x} active layers.

Various active layers and configurations were examined during experiments. We also have deposited additional layer of titanium nitride between active layers of titanium dioxide (Figure 2).

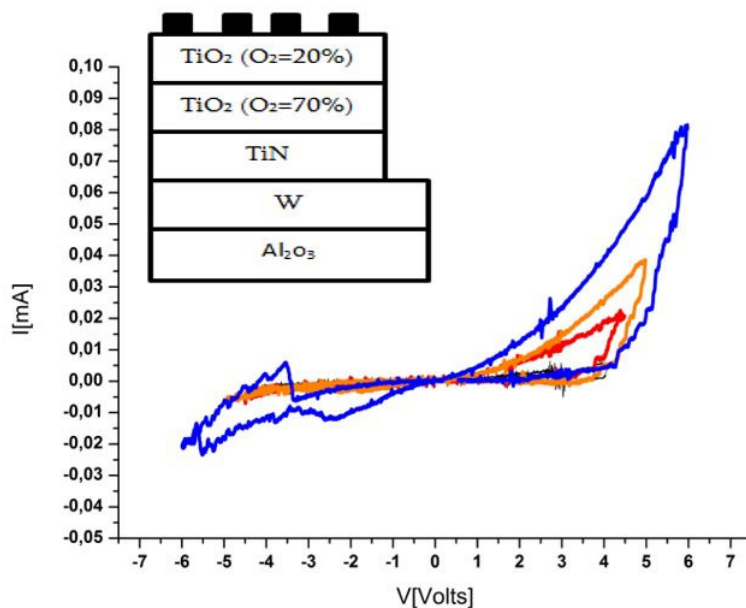


Figure 2. Memristor with TiN layer and its current-voltage characteristics.

Current–voltage characteristics revealed that additional layers have a big influence on hysteresis of memristor. Its characteristics depend on sequence of active layers too. X-ray spectrum has been recorded for all layers of memristor. Voltage–capacity measurements have also been carried out. Absorption and reflection spectra were recorded for all layers.

References

- [1] L. O. Chua. Memristor – The missing circuit element. *IEEE Trans. Circuit Theory*, 1971, 18, 5, 507.
- [2] D. B. Strukov, G. S. Snider, D. R. Stewart, R. S. Williams. The missing memristor found. *Nature*, 2008, 453, 80.
- [3] J. Kwon, A. A. Sharma, J. A. Bain, Y. N. Picard, M. Skowronski. Oxygen vacancy creation, drift, and aggregation in TiO₂-based resistive switches at low temperature and voltage. *Adv. Funct. Mater.*, 2015, 25, 2876.

COORDINATION POLYMERS WITH Cd_2Ln CORES AS BASIS FOR MAGNETIC LUMINESCENT NANOMATERIALS

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Coordination compounds, which combine non-trivial magnetic properties (such as behavior of single molecule magnets or SMM) and luminescence, are considered as a basis for new multifunctional nanomaterials. The aim of this study was to develop methods for preparation complexes, containing Ln(III) and Cd(II) ions in one polynuclear core, and to reveal the influence of Ln(III) ions and carboxylate ligands on the properties of such systems.

A series of isostructural coordination polymers $[\text{Cd}_2\text{Ln}(\text{Piv})_7(\text{H}_2\text{O})_2]_n$, where $\text{Ln}^{\text{III}} = \text{La}, \text{Sm}, \text{Pr}, \text{Gd}, \text{Tb}, \text{Er}, \text{Dy}, \text{Ho}$, Piv = pivalate, and their analogues $[\text{Cd}_2\text{Ln}(\text{hobz})_7(\text{H}_2\text{O})_2]$ ($\text{Ln}^{\text{III}} = \text{Dy}, \text{Nd}$, hobz[−] = 4-n-heptoxybenzoate) was prepared (**Figure 1**; asterisks on the figure indicate atoms of the adjacent $\text{Cd}_2\text{Ln}(\text{Piv})_7(\text{H}_2\text{O})_2$ units). Magnetization of $[\text{Cd}_2\text{Ln}(\text{Piv})_7(\text{H}_2\text{O})_2]_n$ ($\text{Ln}^{\text{III}} = \text{Dy}, \text{Ho}, \text{Tb}, \text{Yb}$) was measured in temperature range 2 – 300 K in direct and alternating magnetic fields. Slow magnetic relaxation was found for $\text{Ln}^{\text{III}} = \text{Dy}$ and Yb, which is typical for SMMs. Ln^{III} -centered emission was found in the luminescence spectra of $[\text{Cd}_2\text{Ln}(\text{Piv})_7(\text{H}_2\text{O})_2]_n$ and $[\text{Cd}_2\text{Ln}(\text{hobz})_7(\text{H}_2\text{O})_2]_n$. Luminescence intensity of $[\text{Cd}_2\text{Dy}(\text{Piv})_7(\text{H}_2\text{O})_2]_n \cdot n \text{CH}_3\text{CN}$ was 5 times higher compared to $[\text{Cd}_2\text{Dy}(\text{hobz})_7(\text{H}_2\text{O})_2]_n \cdot n \text{CH}_3\text{CN}$; this difference could be caused by higher dissipation of the exciting energy in 4-n-heptoxybenzoates compared to pivalates.

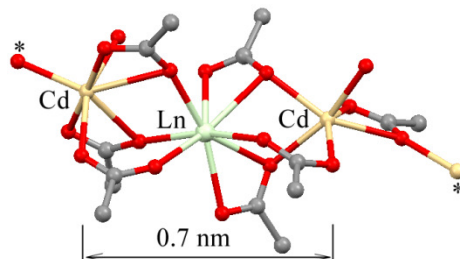


Figure 1. Fragment of polymeric chain of $[\text{Cd}_2\text{Ln}(\text{Piv})_7(\text{H}_2\text{O})_2]_n$ (methyl groups of pivalates are omitted for clarity).

This work was supported by the VolkswagenStiftung, Trilateral Partnership Project “Multifunctional Molecular Materials – Bridging Magnetism and Luminescence”.

ROLE OF INTERFACES IN SPIN DYNAMICS AND FLOWS IN MAGNETIC NANOSTRUCTURES WITH NORMAL METAL SUBLAYERS

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The interconnection between the spin current and spin dynamics via the spin-dependent scattering and accompanying by spin torque effect in ferromagnetic (F) / normal (N) metal based magnetic multilayer nanostructures is studied including a high fast out-of-equilibrium spin dynamics. Features of the spin transport through interfaces and its impact on spin dynamics are described on the base of the scattering matrix formalism for spin flows. The dependence of the spin torque effect on conductance character of the normal metal layers is considered. The exchange processes between the itinerant and the localized electrons are described by kinetic rate equations for electron-magnon spin-flop scattering.

It is shown that the relaxation of the out-of-equilibrium spin accumulation among itinerant electrons provides the principal channel for dissipation of spin angular momentum from the combined electronic system.

The spin-transfer-induced torques on the magnetic moments of $F/N/F$ systems caused by a flowing current has described in the framework of the scattering matrix formalism. This description deals with the effects of multiple scattering between the layers using the scattering matrices of the $F|N$ interfaces as input parameters. Both the cases of a diffusive and ballistic normal metal spacer are considered. In the diffusive case, the high-dimensional scattering matrices of the $F|N$ interfaces only appear through the averaging over the normal metal layers. This allows making qualitative predictions about the role of the interface transparency, normal metal resistance, etc. without detailed knowledge of the microscopic details of the system.

The description has focused on the effects of “spin filtering” as the mechanism for current-induced torque, i.e., the difference in the transmission and reflection probabilities for electrons with spins parallel and antiparallel to the moments of the ferromagnetic. A different source of spin-dependent scattering related to spin-flip scattering is described by the off diagonal terms in the scattering matrices.

The concepts of transverse spin diffusion in bulk ferromagnets and the interfacial spin-mixing physics [1, 2] have extended to address the ultrafast spin dynamics observed in rapidly heated magnetic heterostructures.

In the ultrafast regime, the relative importance of the bulk scattering and the interfacial scattering can be extracted from measurements of demagnetization strength and spin currents in magnetic heterostructures. For metallic ferromagnets in the bulk, treating the magnonic subsystems as quasi-equilibrated and parametrized by an effective temperature is insufficient to describe the far-from-equilibrium spin dynamics induced by pulsed laser heating.

The magnon distribution function remains nonthermalized on the relevant time scale of the demagnetization process, in which the relaxation of the out-of-equilibrium spin accumulation limits the dissipation of spin angular momentum from the combined electronic system.

References

- [1] X. Waintal, E. B. Myers, P.W. Browver, D. C. Ralph. Phys. Rev. B, 2000, 62, 12317.
- [2] E. G. Tveten, A. Brataas, Y. Tserkovnyak. Phys. Rev. B, 2015, 92, 180412.

STABILITY OF SONICATED GRAPHENE OXIDE AQUEOUS SOLS

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Nowadays graphene oxide (GO) is used in various fields due to its good solubility, low toxicity, high surface area in addition to photoluminescence properties, thermal conductivity, etc. GO is a hydrophilic material where the ratio of hydrophilic functional groups to hydrophobic graphene sheets varies with the sheet size. It is important to prepare smaller GO sheets, which results in more stable colloidal dispersions due to higher hydrophilicity.

A lot of different methods were used to increase the solubility of the GO [1, 2]. It is known that upon sonication GO sheets could be cut into smaller pieces. Size distribution of GO sheets can be narrowed to some extent by modifying the preparation conditions.

In this work, we have investigated relation between stability of GO water sols and their lateral dimensions during re-dispersion by sonication. Ultracentrifugation was applied after sonication process to separate the GO fractions.

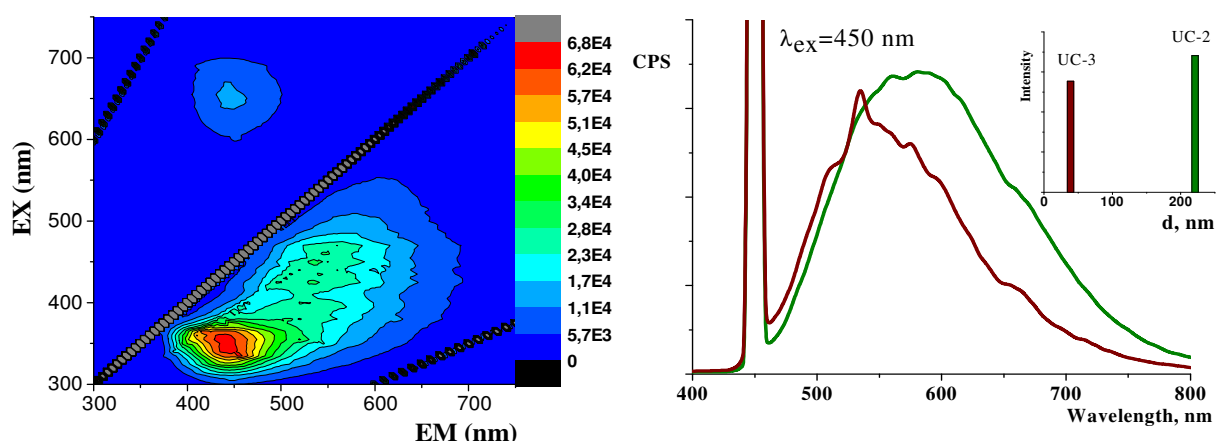


Figure 1. PLE map of GO–UC1 sols and PL spectra GO–UC2, GO–UC3 with their DLS data.

According to TEM data, initial GO (supplied by graphitene) has average lateral particle size close to 400nm. Subsequent ultrasonic re-dispersions of GO (5 mg / ml in water) resulted in increase of intensity of visible range PL of the sols and appearance of a small peak of two-photon PL. Hydrodynamic diameter of particles in the re-dispersed sol (GO–UC2) measured by DLS was reduced by half up to 175 – 250 nm.

Prolonged contact of the GO with water (GO-UC3) resulted in a critical reduction of particle size to (50 nm by DLS) and increased stability of the sols. At the same time the sol GO-UC1 was unstable and formation of aggregates was observed after two weeks. Future studies targeting to improve the stability and dispersibility of GO nanoparticles are planned.

References

- [1] H. Geng, B. Yao, J. Zhou, K. Liu, G. Bai, W. Li, Y. Song, G. Shi, M. Doi, J. Wang. Size fractionation of graphene oxide nanosheets via controlled directional freezing. *J. Am. Chem. Soc.*, 2017, 139, 12517-12523.
- [2] E. Bidram, A. Sulistio, A. Amini, Q. Fu, G. G. Qiao, A. Stewart, D. E. Dunstan. Fractionation of graphene oxide single nano-sheets in water-glycerol solutions using gradient centrifugation. *Carbon*, 2016, 103 363-371.

USE OF DIPOLE ANTENNA IN MICROWAVE RADIOMETRY

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The work is dedicated to the use of dipole antenna in microwave radiometry, which plays a major role in medical diagnostic surveys by determining the dielectric properties of the tissue and its temperature noninvasiveness.

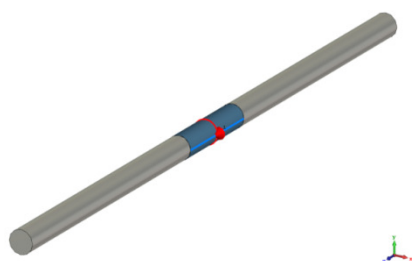


Figure 1. Dipole antenna.

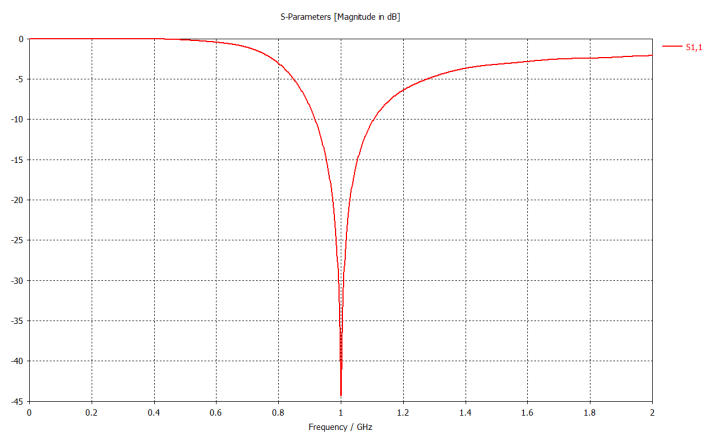


Figure 2. Determination of dipole antenna frequency and magnitude.

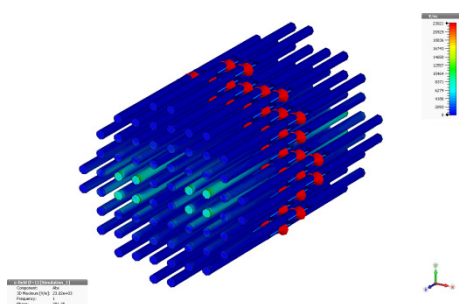


Figure 3. Set of dipole antennas.

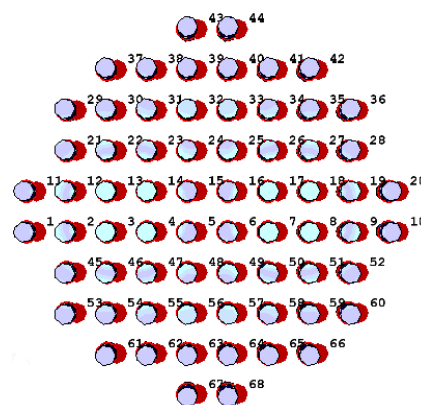


Figure 4. Layout of dipole antennas.

**TO KINETICS OF QUANTUM DISSIPATIVE SYSTEMS
INTERACTING WITH BOSON FIELD: QUANTUM
BROWNIAN PARTICLE MOTION AND LOW
TEMPERATURE POLARON MOBILITY PROBLEM**

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New, exact generalized quantum evolutionary (kinetic) equations for the equilibrium double-time correlation functions (Green's functions: advance, advanced, retarded and casual) and statistical operator (density matrix) of a quantum dynamic system interacting with a phonon (boson) field were derived in the case of linear as to the Bose-amplitudes. The random phase approximation (RLA, factorizing initial condition) has not been used to derive these equations. In the initial moment of time for the correlation functions a thermal initial conditions were used. The projection operator technique and the generalized Bogolubov's lemma for a dynamical system interacting with the Boson field is proved and used for excluding the dynamical variables of the boson field (Boson amplitudes) from the derived evolutionary equations. The collision integrals of these equations include explicitly both the dissipative terms describing the dynamics of the system and the terms responsible for the time evolution of initial correlations.

The derived kinetic equations are used to analyze the kinetic and linear transport phenomena in exactly soluble model of the quantumdissipative system: A quantum Brownian particle dynamics of which is described by the Caldeira–Legget Hamiltonian. The specific form of kinetic equations are obtained and the influence of the initial correlations are discussed. The relaxation time of the correlation functions and the mobility of the Brownian particle were calculated.

As an application of this approach, the uniform theory of Froechlieh's polaron mobility and conductivity, in the wide range of frequency of the weak external field, is developed as well. It reproduces the generalized Osaka result at low frequencies of external electric field and generalized Feynman–Hellwarth–Iddings–Platzman (FHIP) result at high frequencies. Such an uniform theory of low-temperature polaron mobility was not yet developed until.

**CASE STUDY ON VERTICAL MIGRATION OF ^{137}Cs
RADIONUCLIDE IN SOIL OF TWO RESORTS OF GEORGIA
AFTER 31 YEARS FROM CHERNOBYL ACCIDENT**

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The work studies the problem of vertical migration of ^{137}Cs radionuclide in the soil of two Georgian resorts – Ureki and Bakhmaro – located at different height from the sea level after 31 years from Chernobyl accident. The samples were gathered in July, 2017 after the period of one half-decay of the mentioned radionuclide. The great interest to ^{137}Cs problem is caused by its physical-chemical properties, being the reason of the investigation of its migration in the soil. The samples of soil in both places were taken on one and the same day (15.07.17) in the different depths of soil: (the surface is denoted by 0) 0; 10; 20; 30, 40 cm. For investigated two different types of soil the different character of vertical migration of ^{137}Cs radionuclide is clearly seen (**Table 1**).

Table 1. Content of ^{137}Cs radionuclide in the soil of Ureki and Bakhmaro resorts at its vertical migration.

#	Soil depth, cm	Content of ^{137}Cs in soil, Bq / kg	
		Ureki	Bakhmaro
1	0	12.52	24.88
2	10	24.42	13.57
3	20	12.22	1.72
4	30	5.70	–
5	40	4.00	–

SURFACTANTS AND THEIR FUNCTIONS ON NANO-POWDER SYNTHESIS

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Nanoparticles have been drawn attention more than 20 years and this interest looks like to continue in near future. Their unusual properties such as large specific surface area, high chemical reactivity, physical affinity and interesting optical, electrical and magnetic properties has stimulated the researchers to use them in wide range of applications as powders, composite or metal forms. Synthesis of nanomaterials with controlled morphology, size, desirable chemical composition and crystal structure, and finally in large quantity, are the key steps toward nanotechnological applications.

Table 1. Feature sizes for significant changes in properties reported in nanocomposite systems.

Properties	Feature size, nm
Catalytic activity	< 5
Making hard magnetic materials soft	< 20
Producing refractive index changes	< 50
Producing super paramagnetism and others electromagnetic phenomena	< 100
Producing strengthening and toughening	< 100
Modifying hardness and plasticity	< 100

Synthesis of nanoparticle is complex processes. There are three main categories of nanoparticle synthesis and these are vapor phase, solution precipitation and solid-state processes. Although all the three are widely used in practice, the more common process is solid state. In solid state synthesis of nanoparticles generally heat treatment followed by milling is carried out to get an average particle size of 100 nm or less. Mechanical milling or alloying applied at dry or wet form is one of the most preferred and earliest technique to produce nano-sized powders. However, the stabilization of particles and disturbing them in homogenous arrangement is the common challenge to increase the efficiency of milling and to obtain required grain size. Most of the synthesis routs, these are act as important factor to develop the product with desirable properties.

Therefore, in the last years, a broad range of techniques in chemistry and physical chemistry has been offered to stabilize inorganic nanoparticles or to self-assemble them in a controlled manner. The use of surfactants as the stabilizing agents in the preparation of nano powders has been exploited for the synthesis of various nanomaterials, inter-metallic compounds and ceramic nanocomposites from solid state. Self-assembled structures of surfactants act as cationic, anionic or charge neutral lubricants to control the nano / microenviroment of the nanostructured materials, producing nanoparticles with improved

dispersion. Process control agents (surfactants-PCA) are added to the powder mixture during milling to reduce the effect of agglomeration. The PCA adsorbs on the surface of the powder particles and minimizes agglomeration and lower the surface tension of the solid material. A reduction in surface energy results in the use of shorter milling times and / or generation of finer powders. The surfactant coating on nanoparticles changes their aggregation behavior due to changed interparticle potential. Therefore, different types of surfactants, depending upon their molecular structures, may tune the interparticle interactions to different extent and hence have different tendency to prevent the nanoparticles aggregation. Apart from the synthesis purpose, surfactants have been used in association with nanoparticles for variety of studies.

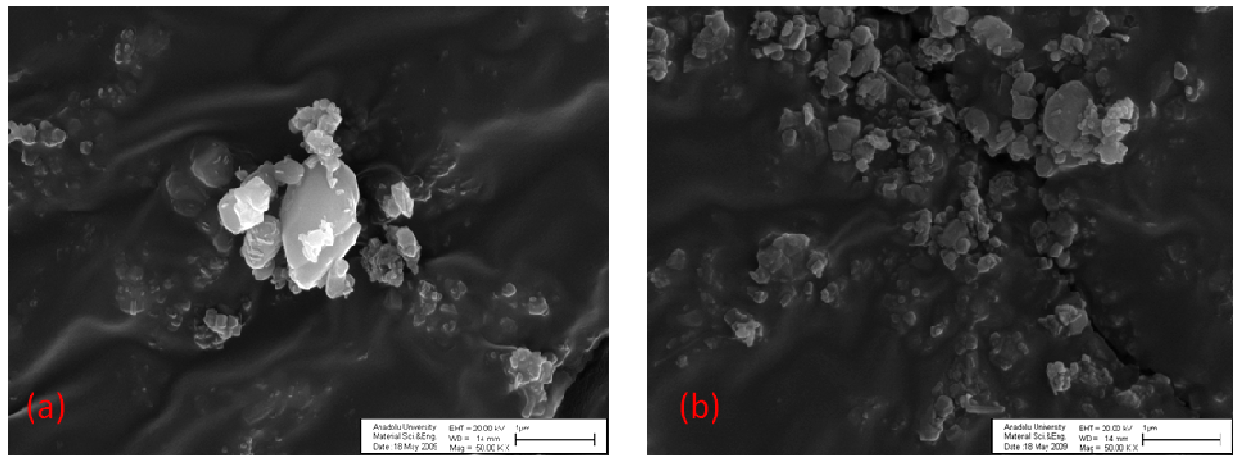


Figure 1. Morphology of β -SiAlON samples conventional (a) and surfactant assisted milled (b) at 20 h.

In this review, the fundamental concept, properties of surfactants and their use in nano powder synthesis are systematically presented. The special attention is given to investigation of medium effect in high-energy ball milling for nitride based powders systems and how does the surfactant usage affects the surface morphology and topological properties of MgB_2 synthesized by solid-state process.

References

- [1] H. Gleiter. Nanostructured materials: Basic concept and microstructure. *Acta Mater.*, 2000, 48, 1-29.
- [2] B. S. Murty, S. Ranganathan. Novel materials synthesis by mechanical alloying / milling. *Int. Mater. Rev.*, 1998, 43, 101-141.
- [3] P. Balaz, E. Godocikova, L. Krilova, P. Lobotk, E. Gock. Preparation of nanocrystalline materials by high-energy milling. *Mater. Sci. Eng. A*, 2004, 386, 442-446.
- [4] P. H. C. Camargo, K. G. Satyanarayana, F. Wypych. Nanocomposites: Synthesis, structure, properties and new application opportunities. *Mater. Res.*, 2009, 12, 1-39.

SOLID-PHASE SPECTROPHOTOMETRIC DETERMINATION OF TRACES OF CATIONIC POLYMERIC FLOCCULATING AGENTS IN TAP AND SURFACE WATER

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Nowadays there is a problem of trace FA determination in water, because of a standard photometric method with eosin (or eosin-Cu(II)) is not sufficiently sensitive. Besides it is not selective. The aim of our researches is to develop the new method for FA with improved metrological characteristics on the base of solid phase photometric determination (diffused reflection spectrometry) after colored complexes preconcentration on the membrane filters.

New method for the determination of the polyhexamethyleneguanidine (PGMG), PolyAmines (FLOQAT™ FL17, FL 28), PolyDADMAC (FLOQAT™ L45) has been created. Procedure is based on complexation of Bromopyrogallol Red with Mo (VI) and FA at pH 0.5 – 1.0; the reaction may be used in two different mode – for photometric determination of FA in water solution (in presence of nonionic surfactants in micellar concentration) and for the solid-phase spectrophotometric determination after colored complexes sorbtion on the membrane filters. The range of FA concentrations that are determined by these procedures are: 0.1 – 10.0 and 0.01 – 0.15 mg / dm³, respectively.

The optimal conditions of FA's complexation in solution and of preconcentration stage have been investigated – pH, concentration of reaction compounds as well as their mixing order, materials of membrane and their pore size, speed of filtration.

The effect of the concentration of PGMG on the diffuse reflection coefficients of colored membranes at 610 nm (λ_{\min}) has been studied. The calibration curve has been obtained for each of above mentioned FA in coordinates $Y - C_{\text{FA}}$, where $Y = F(K_{\text{ref}}) = (1 - K_{\text{ref}})^2 / 2 K_{\text{ref}}$, K_{ref} – diffuse reflection coefficient. The range of FA concentrations that are determined by the proposed procedure are 0.01 – 0.20 mg / dm³; relative errors are < 20 %, the duration of analysis is 15 – 17 min. The color scale for visual determination has been constructed in the working range 1 – 15 µg per sample. Components of drinking and natural water, especially humic substances, do not interfere. This conclusion is confirmed by data; the recovery of added PGMP concentration in river water samples with different "color" and "oxidizability" has been determined by two methods – with eosin and BPGR. When the concentration of natural organic substances (mainly humic substances) increases, the recovery of PGMG by standard method decreases from 80 to 3 – 5 % ; in the same samples the recovery of PGMG by proposed method is equal to 95 – 102 %.

The new method coupled with standard photometric method with eosin has been applied to study the *speciation* of PHMG in real river water samples; it has been found that PHMG and other FA can exist in surface water in two forms - as «free» compounds and as associates with humic acids.

SELENIUM NANOPARTICLES: FLUORIMETRIC DETERMINATION IN WATERS SOLUTIONS USING ANION-EXCHANGING SORBENTS

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In natural waters selenium is contained in different chemical forms each one characterized by respective accessible and toxicity. Therefore, one of the main tasks of the analysis is revealing the various forms of selenium. When determining selenium in waters at the microgram level it is necessary to use a highly sensitive method.

The fluorimetric method is characterized by high accuracy and the low detection limit (DL). It is based on interrelation selenite-ions and 2,3-diaminonaphthaline concurrently with the formation of 4,5-piazselenole, whose optical characteristics are measured on a fluorimeter.

The analysis is substantially simplified by the separation of various valence forms of selenium at the stage of preliminary sorption concentration. Strong-basic anion-exchangers AV-17, daurex, KhAD-4, KhAD-16, KhAD-7NR, ARA-5p in chloride, hydroxide, and acetate forms. Maximum sorption (92 %); observed when using anion-exchanger AV-17 in the acetate form. Therefore, further research was carried out with this sorbent.

We studied the sorption of selenate- and selenite-anions on strongly basic anion-exchanger AV-17 within pH range 7 – 4. It was found that the impact of the concentration of hydrogen ions within pH range 7 – 4 on the degree of extracting inorganic selenium is small, while at further reduction of the pH from 4 to 1 sorption of anions substantially decreases. For maximum extraction of ions sorption is carried out at the neutral pH ~ 7.

For desorption of selenate and selenites solutions of chloride acid of various concentrations were used. It was found that quantitatively desorption of anions is carried out by the solution of chloride acid with the concentration respectively 0.1 and 5 mol / dm³ for 20 min. Fractionation of anions by washing out with the solutions with different acidity is explained by difference in the values of constants of equilibrium of selenate and selenite acids.

The recovery of Se(VI) was carried out during heat treatment of a sample with the concentrated chloride acid. It was found that the most complete recovery of Se(VI) to Se(IV) is achieved when heating a sample with a 5 M of chloride acid.

Correctness of determining selenium was assessed by the method of "introduced-found". The graduation graph is linear within the interval of concentrations 0.1 – 5 µg / dm³. The proposed method during detection by the fluorimetric method makes it possible to determine inorganic selenium at high accuracy ($P = 0.95$) and reproducibility ($S = 2.3$ %) within the wide range of concentrations.

RECEIVING NEW TRIBOLOGICAL POLYTETRAFLUOROETHYLENE-BASED COMPOSITE MATERIALS AND RESEARCH THEIR PROPERTIES

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The research object was receiving new composite materials of polytetrafluoroethylene using natural mineral – chalcopryrite (CuFeS_2) microparticles and research their properties.

On polytetrafluoroethylene (PTFE) base the polymeric composites filled with 2, 5, 5 and 10 wt. % chalcopryrite powder were made.

The research goal is to determine the wear intensity of the composites at different friction speeds, and compare the results to the indicators of the best tribotechnical material “superfluvis”. In case of improving the tribological properties, we will get quite cheap and effective tribotechnical material.

FULLERENE-BASED COMPLEXES IN SOLUTIONS FOR ANTICANCER THERAPY: STRUCTURE CHARACTERIZATION AND TOXICITY TESTS

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Applications of fullerene water solutions (FWS) in medicine and cosmetics [1, 2] are of current interest due to their antioxidant, antitumor and antibacterial properties. However, there is no consensus to the question about influence of these systems in living organisms so far. In the literature both positive and negative health influences have been reported depending on the type of primary organic solvents used in the technique preparation and the cluster size distribution in the final solutions, as well as on the chemical modification of fullerenes resulting in a wide class of biologically active derivatives. In particular, there are indications [3] that cytotoxicity and antibacterial properties of FWS correlate with the aggregate formation. The latter also has an impact on the environment, since after utilization the FWS interacting with natural salts coagulate, which significantly complicates their removal.

The presented paper is devoted to the comparison of the efficiency of fullerene C₆₀ water solutions with respect to their application for the treatment of oncological diseases. Different methods of preparation of fullerene water solutions were considered. At the initial stage of research, the detailed structure analysis for each solution in water and after fullerene transfer in saline solutions included several methods (small-angle X-ray and neutron scattering, dynamic light scattering, atomic force microscopy, transmission electron microscopy, UV-Vis spectroscopy). At the next stage, cytotoxicity *in vitro* tests with mammalian fibroblasts of Chinese hamsters, line V-79, revealed good survival at fullerene concentrations up to 5 µg / ml. Subsequent investigations of the complexation of fullerenes with several anticancer drugs for potential enhancement of their activity concerned were presented.

References

- [1] E. Oberdorster, Manufactured nanomaterials (fullerenes, C₆₀) induce oxidative stress in the brain of juvenile largemouth bass. *Environ. Health Perspect.*, 2004, 112, 1058-1062.
- [2] F. Moussa. Fullerene is an *in vivo* powerful antioxidant with no acute or sub-acute toxicity. *Nano Lett.*, 2005, 5, 2578-2585.
- [3] D. Y. Lyon, L. K. Adams, J. C. Falkner, P. J. Alvarez. Antibacterial activity of fullerene water suspensions: Effects of preparation method and particle size. *Environ. Sci. & Technol.*, 2006, 40, 4360-4366.

MAGNETIC PROPERTIES OF AURUM-BEARING NANOPARTICLES FORMED ON STEEL SURFACE UNDER ROTATION-CORROSION DISPERSION CONDITIONS

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The rotation-corrosion dispersion (RCD) method based on simple red-ox reactions that including anodic dissolution of an iron-bearing component in the steel composition and oxygen depolarization in a cathodal part of the steel surface. Development of the primary iron-oxygen particles on the steel surface carried out from metastable Fe(II)–Fe(III) layered double hydroxides (green rust) to lepidocrocite, goethite or magnetite. The presence of precious metal aqua forms leads to the formation of the core & shell type nanoparticles that usually form ionic-stabilized sols. Under the following conditions green rust plays the role of a strong reducing agent. Whereas ferric oxyhydroxides can occlude (adsorb) the precious metal ions without red-ox reactions, magnetite nanoparticles, in the presence of aurum species, simultaneously take part in reducing and sorption processes. We suppose that the magnetic properties of the iron-oxygen nanostructures obtained via the RCD route can be changed due to the influence of the dissolved aurum species. The magnetic properties of the aurum-bearing nanopowders were studied versus a synthesis temperature, initial concentrations of aurum aqua forms, and a phase composition of primary iron-oxygen structures, preliminary formed on the steel surface. In general, all as-synthesized samples did not show remanence magnetization M_r and coercitivity H_c . The shape of hysteresis loops was indicative for superparamagnetic nanoparticles. Whereas the saturation magnetization of the sample obtained at $T = 50\text{ }^{\circ}\text{C}$ equaled $14\text{ A} \cdot \text{m}^2 \cdot \text{kg}^{-1}$, the reduction of the synthesis temperature up to $T = 20\text{ }^{\circ}\text{C}$ led to decrease of M_s to $2\text{ A} \cdot \text{m}^2 \cdot \text{kg}^{-1}$ and it resulted in disappearance of a hysteresis loop. The role of the aurum concentration on the saturation magnetization of the surface structures was studied in the wide range of $c\text{Au}^{3+}$ (from 0.02 to $1.0\text{ g} \cdot \text{dm}^{-3}$). According to the obtained data the values of M_s gradually grew from 14 to $40\text{ A} \cdot \text{m}^2 \cdot \text{kg}^{-1}$ when the initial Au^{3+} concentration was increased from 0.02 to $0.5\text{ g} \cdot \text{dm}^{-3}$. But the parameter M_s sharply fell to $4\text{ A} \cdot \text{m}^2 \cdot \text{kg}^{-1}$ at $c\text{Au}^{3+} = 1\text{ g} \cdot \text{dm}^{-3}$. In the latter case the hysteresis loop had a disturbed mode. So, we supposed the appearance of the second nonmagnetic aurum-bearing phase, not excluding. So, gold nanoparticles, at Au^{3+} concentration $0.05\text{ g} \cdot \text{dm}^{-3}$ the parameter M_s gradually increased from 18 to 25 and further to $30\text{ A} \cdot \text{m}^2 \cdot \text{kg}^{-1}$, when the nonoxidized steel surface was covered by the hydroxycarbonate green rust layer and green rust was transformed into lepidocrocite phase, respectively. But at the concentration $\text{Au}^{3+} = 0.5\text{ g} \cdot \text{dm}^{-3}$ the value of M_s was higher ($40\text{ A} \cdot \text{m}^2 \cdot \text{kg}^{-1}$), except of the sample obtained in the presence of green rust precursor where such parameter decreased to $14\text{ A} \cdot \text{m}^2 \cdot \text{kg}^{-1}$.

PHYSICAL-CHEMICAL PROPERTIES OF NANOSIZED SPINEL FERRITE NANOPARTICLES FORMED VIA ROTATION-CORROSION DISPERGATION ROUTE

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The possibility to obtain the nanosized spinel ferrite nanoparticles on the surface of the steel electrode under the rotation-corrosion dispergation (RCD) conditions strongly depends on the chemical compositions and pH value of the dispersion medium contacting with the steel surface, temperature and duration of the phase formation process [1]. Other determinative factor is the presence of primary species on the electrode surface. The experimental modeling of the RCD process in the cobalt-, nickel-, zinc- and copper-containing water salt solutions pointed out that the colloid-chemical mechanism of the spinel ferrite formation lied in the chemical interaction of ferric / ferrous and corresponding 3d-metal aquahydroxoforms on the steel surface, whereas the solid-state transformation of the preliminary formed green rust or lepidocrocite particles was not confirmed [2]. Generally, the anion composition of the dispersion medium influences the phase composition of the surface structures. So, the main mineral phases obtained in the chloride-containing medium are spinel ferrites and ferric oxyhydroxides, typically, lepidocrocite. The sulfate-containing solution contacting with the steel surface promotes the appearance of the mixed Me(II)–Fe(III) layered double hydroxides, but only spinel ferrite particles are formed in the nitrate-containing solutions. The type of cations of the dispersion medium influences the mechanism of cation fixation by the spinel ferrite structure. Whereas Co^{2+} is included into spinel ferrite crystal lattice, Cu^{2+} , Zn^{2+} and Ni^{2+} are adsorbed on the surface of the iron–oxide nanoparticles and may be easily removed from the particle's surface in the acidic water solutions via desorption process. In addition, mainly lepidocrocite particles are obtained as a second mineral phase in the presence of zinc cations, but both ferric oxyhydroxide phases (lepidocrocite and goethite) are formed on the steel surface in the presence of nickel, cobalt or copper cations. In addition, the spinel ferrite structures obtained in nickel-, zinc and copper-bearing systems as well as the products of their phase transformation due to the thermal treatment in the wide range of temperatures (from 50 to 740 °C) show the superparamagnetic properties, but all structures formed in cobalt-bearing systems demonstrate ferrimagnetic properties [3].

References

- [1] O. M. Lavrynenko, O. Yu. Pavlenko, Yu. S. Shchukin. *Nanoscale Res. Lett.*, 2016, 11, 67.
- [2] O. M. Lavrynenko, O. Yu. Pavlenko, Yu. S. Shchukin, P. A. Kosorukov, O. V. Legenchyk. *Mater. Sci. Nanostruc.*, 2014, 2, 18.
- [3] O. Lavrynenko, N. Dudchenko, O. Pavlenko, A. Brik. *Eur. Chem. Bull.*, 2016, 5, 12, 524.

HALL-TYPE THIN FILM SoI NANOTRANSISTORS – BASE OF NEW GENERATION OF SMART Si SENSORS

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The results of physical and TCAD mathematical modeling as well as the experimental investigation of a Si thin film nanotransistors (TFT) with built – in channel and a double gates control system of MISIM (metal–insulator–Si–insulator–metal) type are presented. TFT channel contains two opposite lateralohmic contacts that provides the ability to measure magnetic induction in accordance with the Hall effect.

Such magnetosensitive element (so-called the field effect Hall sensor – FEHS) provides the creation of magnetic sensors and systems with radically improved characteristics and functionality in compare with the traditional Si Hall probe and magnetosensitive IC.

In particular FEHS provides

- multiple increase of threshold magnetosensitivity;
- record the wide range of operating temperatures (from liquid helium up to 500 °C);
- the ability of operate in the accumulation and depletion modes and in the mode of split drain transistor, which essentially extended the range of circuit solution in development of sensor devices;
- possibility to measure and perform frequency spectroscopy of alternative magnet fields;
- using the MISIM system to modulate the channel current and significantly for the purpose of the synchronous detection of the Hall signal and increasing of the signal / noise ratio by orders of magnitude;
- using the MISIM system to organizing feedback from the Hall contacts and controlled gates and / or power supply source for a significant improvement in measurements' stability;
- multiple decrease of operating current;
- increasing the magnetosensitivity due to the effect of charge connection between the control field gates.

The noted advantages of FEHS are due not only of FEHS construction the variability of electronics modes and circuit use but also not least through the use of SoI (silicon-on-insulator) technology for manufacture of FEHS and interface electronics of sensors.

ELECTRODEPOSITION OF TUNGSTEN NANOSTRUCTURED GALVANIC COATINGS FROM TUNGSTATE MELTS

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Electrodeposition of nanostructured tungsten coatings was realized from the electrolytes KCl–NaCl–Na₂WO₄ and Na₂WO₄ with NaPO₃ additives. The influence of variations in the concentrations of Na₂WO₄ and NaPO₃, temperature, cathodic current density, and length of the electrolysis period on the composition and structure of the cathodic deposits were studied. Optimal deposition parameters with current reversal were selected.

Nanostructured tungsten coatings in a KCl–NaCl–Na₂WO₄–NaPO₃ melt were produced once the previously determined relation $0.02 < [\text{PO}_3^-] / [\text{WO}_4^{2-}] < 0.18$ was satisfied. At a Na₂WO₄ concentration less than 1 mole %, the deposit does not exhibit adhesion and phosphide impurities are found in the deposit. At concentrations greater than 10 mol.% the diffraction patterns reveal tungsten oxides. At concentrations of metaphosphate exceeding $[\text{PO}_3^-] / [\text{WO}_4^{2-}] = 0.18$, the tungsten is again released from the phosphides and no adhesive coating is formed.

Nanostructured tungsten coatings in a Na₂WO₄–NaPO₃ melt were obtained at a metaphosphate concentration of from 0.5 to 15 mole %. Above this limit, tungsten bronzes are deposited and the growing deposit rapidly becomes dendritic.

Uniform tungsten coatings fabricated from oxyhalide electrolyte were obtained at Tin the range 973 – 1073 K, and cathodic current density of up to 25 A / dm². Uniform tungsten coatings from oxide electrolyte are obtained at T in the range 1023 – 1123 K and current densities of up to 40 A / dm².

The parameters of the reverse deposition regime were selected for the electrolytes KCl–NaCl–2.5 mol.% Na₂WO₄–0.35 mol.% NaPO₃ and Na₂WO₄–5 mol.% NaPO₃. Adhesive, uniform, nonporous coatings from electrolytes with this composition were obtained at temperatures of 923 and 1173 K and current densities in the ranges 1 – 15 and 3 – 25 A / dm², respectively. The rate of deposition of tungsten in the range of current densities that were studied amounts to 5 – 15 μm / h in oxyhalide electrolyte and 20 – 45 μm / h in oxide electrolyte, and the current yield of tungsten in the form of a coating amounts to 60 and 95 %, respectively.

An attempt was made to avoid production of a coarse-grained structure through use of a reverse electrolysis regime. The ratio of the length of the cathodic period to the anodic one varied from 15 to 50, the anodic period from 0.5 to 3.0 s, and the anodic current density from 20 to 50 A / dm². For the electrolyte Na₂WO₄–5mole%NaPO₃ with $T = 1173$ K, the optimal parameters were $i_c = 15$ A / dm², $i_a = 30$ A / dm², $\tau_c = 25$ s, and $\tau_a = 1.5$ s. As a result, it was possible to create comparatively smooth coatings up to 0.5 mm in thickness on the cathode.

SYNTHESIS OF NANOSTRUCTURED COATINGS MOLYBDENUM (TUNGSTEN) – NICKEL (COBALT) IN TUNGSTATE MELTS

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The addition of molybdenum(VI) oxide to the nickel-containing tungstate melt induces the dimolybdate ion reduction wave. The difference in the potentials of nickel and molybdenum deposition is 0.09 – 0.115 V at 1173 K. For the cathodic codeposition of metals to form an alloy, the molybdenum anode was replaced by a more inert nickel electrode, and electrolysis was carried out at cathodic current densities of 0.05 and 0.1 A / cm² in the temperature range 1123 – 1173 K. The concentration of MoO₃ was maintained at 1.0 – 2.5 mole %, and the NiO concentration was varied from 0.1 to 1.0 mole %. Continuous layers of the intermetallics MoNi, MoNi₃, and MoNi₄ are sequentially deposited on the cathode at 1123 – 1173 K from the melts containing 0.1 – 1.0 mole % NiO.

The introduction of tungsten(VI) oxide into a nickel-containing tungstate melt produces the ditungstate ion reduction wave. The difference in the potentials of nickel and tungsten deposition is 0.13 – 0.16 V at 1173 K. In this case, the deposition dependences are similar to those obtained for the Mo–Ni alloys. The addition of tungsten(VI) oxide to a cobalt-containing tungstate melt results in the appearance of the ditungstate-ion reduction. The difference in the potentials of cobalt and tungsten deposition is 0.08 – 0.14 V at 1173 K. Continuous layers of the CoW and Co₃W intermetallics are sequentially deposited on the cathode at 1123 – 1173 K from the melts containing 0.1 – 1.0 mole % CoO.

The addition of molybdenum (VI) oxide to the cobalt-containing tungstate melt induces the dimolybdate ion reduction wave. The difference in the potentials of cobalt and molybdenum deposition is 0.06 – 0.110 V at 1173 K (cobalt is more inert than molybdenum). These dependences of electrodeposition of tungsten–cobalt alloys are also characteristic of the deposition of molybdenum–cobalt alloys. Depending on the ratio of the MoO₃ and CoO concentrations and the cathodic current density, continuous deposits of Mo, CoMo, Co₃Mo, and Co can be prepared from a Na₂WO₄–MoO₃–NiO melt.

Molybdenum(tungsten)–nickel(cobalt) alloys and intermetallics can be deposited as continuous nanostructure layers on a cathode from oxide melts. The composition and structure of the deposits can be controlled by varying the concentration of the corresponding components in the melt, the temperature, and the cathodic current density. An increase in the nickel(cobalt) content in an alloy with an increase in its concentration in the melt, a decrease in the cathodic current density, or an increase in the electrolysis temperature are most likely due to an increase in the fraction of the total current consumed to deposit nickel(cobalt) and to a decrease in the diffusion retardation for the ions of the more electrochemically negative component of the alloy.

SYNTHESIS OF Co_3O_4 THIN FILMS BY SILAR METHOD AT DIFFERENT SUBSTRATES

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Cobalt oxide thin films are versatile materials due to their industrial applications. It is widely used as supercapacitor, gas sensor, anode electrode in Li-ion batteries, etc. [1]. Co_3O_4 thin films were prepared by different techniques such as chemical bath deposition, sol-gel process, pulsed laser deposition, successive ionic layer adsorption and reaction (SILAR) method and spray pyrolysis on variety of substrates. In the present work, Co_3O_4 thin films have been deposited using SILAR method on glass and silicon wafer substrates.

Before the growth process, the glass substrates were cleaned in dilute HCl solution, rinsed in distilled water: ethanol acetone (1 : 1) mixture and dried in oven at 100 °C. The silicon substrate was etched in hydrofluoric acid (HF) solution to remove native silicon dioxide from wafers, and washed thoroughly with distilled water. Cobalt oxide films were deposited from the cationic precursor of 0.5 M cobalt acetate $[\text{Co}(\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}]$ with 1 M sodium hydroxide solution to make pH ~ 12 and H_2O_2 (3 %) as anionic precursor. The formation process was carried out in 60 cycles and the reaction occurred on the surface forming CoOOH . The deposited films were annealed in air at 300 °C for 3 h to transform the oxyhydroxide phase to the oxide. The Co_3O_4 thin films on glass and silicon substrate were used to study the optical absorption by UV-Vis spectroscopy. The direct optical band gaps for samples synthesized on glass are 1.90 and 3.53 eV; for samples synthesized on silicon substrate is 1.60 eV. The presence of two band gaps can be attributed by ligand-metal charge transfer events: $\text{O}^{2-} \rightarrow \text{Co}^{3+}$ (E_{g1}) and $\text{O}^{2-} \rightarrow \text{Co}^{2+}$ (E_{g2}) [2]. Sizes of the particle identified from the band gap energy are 1.03 and 2.00 nm for glass substrate, and 3.86 nm for silicon substrate. EDX analysis was used to determine the composition of the Co_3O_4 . EDX spectrum for sample synthesized on glass substrate shows that the experimental atomic percentages of Co, O and Si are found to be 14, 58 and 19.5 %, respectively, which is near to the theoretical ratio (3 : 4) of Co_3O_4 .

References

- [1] J. Wollensteina, M. Burgmair, G. Plescher, et al. Sens. & Actuat. B, 2003, 93, 442-448.
- [2] S. A. Makhlof, Z. H. Bakr, K. I. Aly, et al. Superlatt. & Microstruc., 2013, 64, 107-117.

EFFECT OF NANOSTRUCTURES ON PROPERTIES OF HIGH-STRENGTH STEEL WELDED JOINTS PRODUCED BY LASER WELDING

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The nanostructures and phase composition of welded joints of high-strength 14KhGN2MDAFB steel produced by advanced high-speed technologies laser welding have been investigated. Structural-phase changes in the weld metal and in the heat-affected zone were studied by methods of optical metallography and analytical scanning electron microscopy (scanning electron microscope SEM-515 from PHILIPS, The Netherlands) as well as transmission micro diffraction electron microscopy (JEM-200CX, company JEOL, Japan, with accelerating voltage of 200 kV). The executed strength characteristics and distribution of local inner stresses, which are the potential sources of incipience and propagation of cracks in the investigated structural microregions [1 – 5]. As a result of the action of laser welding on the weld metal and the heat affected zone of high-strength steel, a homogeneous dispersed fine-grained structure is formed with a uniform distribution of carbide-type nano-phases in them. The use of high-speed welding technologies allows obtaining structures that provide high operational properties of welded joints.

References

- [1] L. Markashova, O. Berdnikova, A. Bernatskyi, M. Iurzhenko, V Sydorets. Physical and mechanical properties of high-strength steel joints produced by laser welding. In: Young Sci. Forum Appl. Phys. & Eng., 2017, IEEE Int., 88-91.
- [2] L. I. Markashova, V. D. Poznyakov, E. N. Berdnikova, S. L. Zhdanov, V. D. Shelyagin, T. A. Alekseenko. Structure and service properties of hybrid laser-arc welded joints of 14KhGN2MDAFB Steel. Paton Weld. J., 2016, 5-6, 104-113.
- [3] M. I. Gol'dshtein, V. S. Litvinov, B. M. Bronfin. Metallophysics of High-Strength Alloys, 1986, Moscow, Metallurgiya.
- [4] O. N. Romaniv. Fracture Toughness of Structural Steels, 1979, Moscow, Metallurgiya.
- [5] V. E. Panin, V. A. Likhachev, Yu. V. Grinyaeva. Structural Levels of Deformation of Solids, 1985, Novosibirsk, Nauka.

NANO CARBONS HYBRID MATERIALS SYSTEMS FOR ENERGY AND ENVIRONMENT SUSTAINABILITY

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Sustainability is a comprehensive and complex system of systems requiring multidisciplinary and interdisciplinary science and technology inputs with economic, environmental and social objectives. In the last sixty years the global population has grown exponentially from 2.5 to 7 billion people and is expected to continue at an accelerated rate, introducing major and urgent challenges in the energy and environment. Considerable achievements have recently been obtained in the development of nano, nanostructured and nano-hybrid material systems providing significant opportunities for energy and environment sustainability. Due to their exceptional stiffness, strength, thermal and electrical conductivity, carbon nanotubes and graphene have the potential for the development of nano hybrid materials systems for a wide variety of applications. In order to achieve the full potential of carbon nanotubes and graphene for thermal, structural, and electrical applications, carbon nanotubes and graphene need to be developed into bulk fully integrated hybrid materials. Full integration of nanotubes and graphene requires their development beyond conventional composites so that the level of the non-nano carbon material is designed to integrate fully with the nanotubes and graphene. Here the carbon materials are often part of the matrix rather than a differing component, as in the case of conventional composites. The goals are to implement multifunctional nanoarchitectural designs to fully mimic the properties of carbon nanotubes and graphene on larger scales for enhanced thermal and electrical management in addition to the control of other properties such as strength, toughness energy and power. These new approaches involve exfoliation, functionalization, dispersion, stabilization, alignment, polymerization, reaction bonding and coating in order to achieve full integration. Typical examples of thermal and structural applications of polymeric and ceramic matrices and applications in energy systems such as capacitors and batteries as well as other material systems are presented and discussed.

References

- [1] F. D. S. Marquis. Carbon nanotube nanostructured hybrid materials systems for renewable energy applications. JOM, 2011, 63, 48.
- [2] F. D. S. Marquis, L. P. F. Chibante. Improving the heat transfer of nanofluids and nanolubricants with carbon nanotubes. JOM, 2005, 12, 32.
- [3] K.-P. Lee, A. I. Gopalan, F. D. S. Marquis. The nanotechnology of carbon nanotube nanofluids In: Functional Composites of Carbon Nanotubes and Applications (Ed. F. D. S. Marquis), 2009, Research Signpost, ISBN 978-81-7895-413-4.

USE OF NANOCARBON OBTAINED FROM SECONDARY RAW MATERIAL FOR MODIFICATION OF COMPOSITION COATINGS

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Creation of nanostructured modified metal coatings with a multifunctional purpose, having unique thermal, electrical properties, physical and chemical stability is possible by use nanomaterials, because of their specific surface, high porosity and subminiature structure. The achievement of such properties for conventional coarse-grained coatings is impossible.

A group of authors of this work obtained high-quality carbon nanomaterial by thermochemical method of processing worn tyres (United States Patent and Trademark Office, patent no. 9663662) The financing was provided by the private technology company “Long Arc Technologies Corporation”.

New carbonic nanomaterials will be created from different secondary raw material (sawdust, agricultural waste, etc.) by use of acquired experience and knowledge. Nanomaterials obtained from this secondary raw material were tested in galvanic composition coatings. For the purpose of uniform distribution in nickeling electrolyte, the carbonic nanomaterial, in accordance with selected conditions, was dispersed on the ultrasonic disperser. In the obtained solution, the electrolysis was carried out at high temperature (60° C), under the conditions of continuous stirring. Cathodic current output was 90 – 95 %. The structure and composition of composition coating was determined on SEM.

It turned out that some of the elements from carbonic nanomaterial had passed into the nickel composition coating. Experimental studies have shown that physical and mechanical properties have improved in comparison with traditional nickel coating – hardness and strength significantly increased, and sliding and friction coefficient decreased by 2.5 times.

INFLUENCE OF IRRADIATION WITH DEUTERIUM IONS ON MAGNETIC PROPERTIES OF NICKEL

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The magnetic properties of ferromagnets strongly depend on the defectiveness of the crystal structure. This causes the appearance of magnetic hysteresis and magnetic consequences. Irradiated crystals are affected by both dislocations and damage zones. Information on the coercive force H_c makes it possible to judge not only the degree of defectiveness of the ferromagnetic, but also the dominant type of defects and their distribution. The paper considers the evolution of the structure of the nickel surface layer under the action of deuterium ions with increasing radiation dose. The kinetics of structural transformation development in the implantation steel layer was traced from deuterium TDS as a function of implanted deuterium concentration. The sample structure was examined by means of TEM. The magnetic characteristics of nickel were measured with a bar-and-yoke permeameter. It is shown that the formed structure controls the rate and temperature of desorption of the implanted deuterium. Polycrystalline Ni samples with a purity of 99.98 wt. %. Samples look like disks with a diameter of 10 mm and a thickness of 0.05 mm. It is carved from foil, which was annealed. They were fixed in the target device, which cools the sample to 78 K in the dose range from $8.0 \cdot 10^{14}$ to $2.7 \cdot 10^{18}$ D / cm². The samples were irradiated with a beam of ions with an energy of 12 keV.

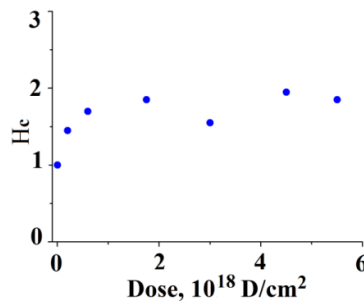


Figure 1. Relative dependence of the coercive force H_c of nickel on dose of implanted deuterium. Coercive force of the initial annealed Ni is taken as unity.

Figure 1 shows the dependence of the coercive force on the dose D of implanted deuterium. When irradiated with a dose of more than $2 \cdot 10^{18}$ D / cm² there are inhomogeneous distribution spectrum of released deuterium that are associated with an increase in non-uniformly distributed defects of radiation origin, such as clusters of dislocations or other local distortions. In the interval up to $2 \cdot 10^{18}$ D / cm², the dependence obeys the law $H_c \sim D^{1/2}$, which agrees well with the rate of accumulation of dislocation groups – $H_c \sim Vn$, where n is the density of these groups. The subsequent of inhomogeneous distribution spectrum of released deuterium in **Figure 1** are due to the development of competing processes of accumulation and relaxation of radiation-stimulated elastic stresses.

FEATURES OF BORON CARBIDE SINTERING PROCESS

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Boron carbide belongs to non-metallic materials commonly referred as ceramic material. B₄C is used in refractory applications due to its high melting point and thermal stability; it is commonly used in nuclear applications as neutron radiation absorbent. B₄C is a premier armor material for personal and vehicle safety due to its low density and high hardness. Nowadays, spark plasma Sintering method has been considered as the most promising method for producing dense bodies of producing pure B₄C ceramics still present problematic task, due to its high sintering temperature 2100 – 2200 °C. At the same time producing B₄C requires long-standing and labor-consuming procedures. Thus, the various additives such as C, Al, Fe, Ti, SiC, TiB₂, Al₂O₃, and ZrO₂ have been used in order to decrease the sintering temperature and improve sintering process. Bulk boron carbide (B₄C) ceramics was fabricated from a boron and carbon mixture SPS [1 – 3]. Densification and synthesis of powder were carried out at the SPS device, which has been designed and built in the Republic Center for Structure Researches (RCSR) at the Georgian Technical University. The developed device for sintering nanocrystalline composite materials was equipped with low-voltage pulsed AC current generators. Graphite molds with special shape was used for synthesise nanopowder of boron carbide. Densification was carried out via graphite press form with standard shape and diameter 12 mm. Nanopowder produces via SPS method were compared with powder synthesized due to carbothermal reaction. Amorphous boron and carbon powders were used as precursors. Without additives nanopowders were produced with pressureless SPS regime at 1600 °C for 5 min. Diffraction peak profile analyses and SEM micrographs detects nanopowder with grain size less than 100 nm. For comparison of dense bodies standard boron carbide has been hot pressed during 2 h under 1900 °C temperature. SPS densification of fully dense samples requires lower temperature and several minutes (1700 °C for 10 min), instead of long-standing and high temperature procedures.

References

- [1] T. K. Roy, C. Subramanian, A. K. Suri. Pressureless sintering of boron carbide. *Ceram. Int.*, 2006, 32, 227.
- [2] X. G. Li, D. Jiang, J. Zhang, Q. Lin, Zh. Chen, Zh. Huang. Densification behavior and related phenomena of spark plasma sintered boron carbide. *Ceram. Int.*, 2014, 40, 4359.
- [3] A. K. Suri, C. Subramanian, J. K. Sonber, T. S. Murthy. Synthesis and consolidation of boron carbide: A review. *Int. Mater. Rev.*, 2010, 55, 4.

DETERMINATION OF SHARE OF ELECTRIC QUADRUPOLE ADMIXTURE FOR ^{169}Tm 93.61 keV γ -TRANSITION

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Studying multipoles of γ -radiation and determination of share of admixture in the case of mixed γ -transition is necessary to study the physical properties of the excited levels of nuclei and to verify different theoretical nuclear models. It is also important to investigate the forms of conversion lines and determine their half-widths. Accumulated quantitative materials give possibility to receive new information about nuclei and atomic levels.

In the paper, the results of investigations of internal conversion electron (ICE) spectrum of ^{169}Tm 93.61 keV γ -transition are presented. Measurements were carried out by means of magnetic beta-spectrometer with 0.04 % high resolution. Forms of L_I , L_{II} , and L_{III} conversion lines are studied and relative amounts of their expansions are measured. Mean quantity of δ^2 from the established internal conversion coefficients (ICC) are calculated $\delta^2 = 0.034 \pm 0.003$. Average significance of the share of electric quadrupole admixture $a = 3.3 \pm 0.3$ % are found, which corresponds to M1+3.3%E2 mixed -transition.

ON PRODUCTION OF HARD NANOCRYSTALLINE MATERIALS

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A technology has been developed for the production of nanocrystalline systems of a wide range – by spraying liquid solutions of salts of the corresponding components with liquid organic compounds into a reactor with a reducing or carbide-forming medium. After pyrolysis, selective reduction processes and carbidization, a powder is obtained, each particle of which can consist of nanocrystalline components (10 – 80 nm, in accordance with the initial solution) – metals, oxides, carbides, quasibinary ceramics.

In this way and by subsequent spark plasma compacting of powders there are obtained:

- Dispersive-strengthened transition metals and alloys, while with retained good plastic properties;
- Nanocrystalline cermets based on titanium-, tungsten-, boron-carbides with high hardness and enhanced strength; and
- Nanocrystalline ceramics based on B₄C–TiB₂ composition with high hardness and increased toughness.

PROSPECTIVES OF HIGH VOLTAGE PULSED ARC DISCHARGE ON NANOMATERIAL SYNTHESIS AND PROCESSING

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Iron oxide nanoparticles (IONPs) are of great interest for researchers working in different fields of physics, chemistry, biology and medicine. Growing interest is based on their physical-chemical and pharmacokinetic properties. Such nanoparticles, in contrast to their volume analogues, exhibit unique features that are widely used in different fields of science and technology, such as electronics, energy, biotechnology and medicine. It is also possible to conjugate them with appropriate molecules of targeted drug delivery for in-vivo studies.

A well-known method of synthesis of IONPs is chemical co-precipitation. Although this method is distinguished by its simplicity, cheapness and the possibility of producing in a large scale, its main drawback is that it is impossible to uniformly distribute the concentrations of reactants, control the nucleation and crystal growing. This ultimately leads to lesser reproducibility and larger polydispersity of the nanoparticles.

The precise control and automation of the synthesis will improve the control over the physical-chemical properties of nanoparticles and the parameters such as mean size and particle size distribution, and the reproducibility of the synthesis.

To do this, we improved our elaborated automated technological line of continuous production [1] by adding an electrohydraulic equipment [2] to process nanoparticles. The proposed approach, as shown by preliminary studies [3], significantly improves the dispersion of solution. Strong oscillations associated with electrohydraulic effect, additionally disperse the chemically synthesized particles. The process is presented as a series of controlled explosions, produced by high voltage electric impulse is charges in the liquid. The discharges generate massive shock waves and impulses of pressure imposing homogenization of the dispersion and lead to increased particle solubility.

In the present work we overview trends of the technique of nanomaterial production and processing by pulsed high voltage discharge in solution/water. Magnetic fluids with citric acid, PEG, PVA-modified magnetite nanoparticles were subjected to 1.2 kV and several hundred nanosecond discharge (**Figure 1**) pulses were investigated.

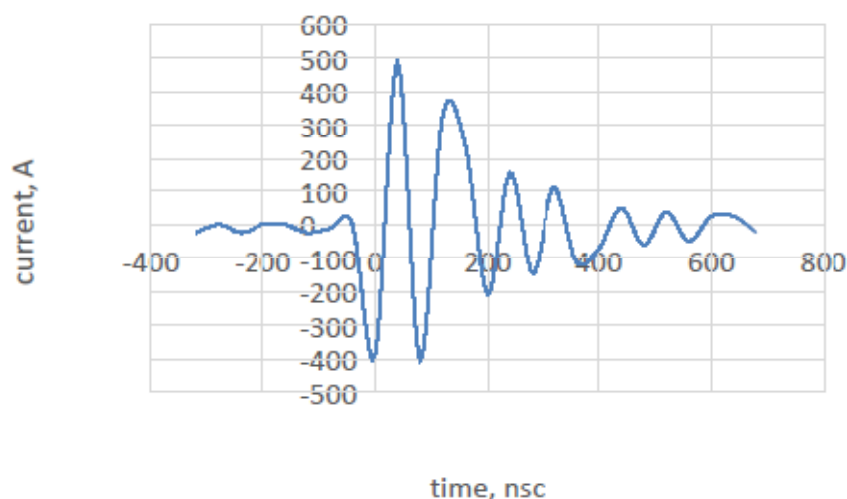


Figure 1. Discharge current of electrohydraulic equipment.

Small-angle neutron scattering (SANS) [4] and small-angle X-ray scattering (SAXS)[5,6] was used for the determination of the microscale or nanoscale structure of particle systems in terms of average particle sizes, shapes, size distribution, and surface-to-volume ratio. Additional information was obtained on the colloidal stability, the quality of the dispersion and the amount and character of the possible particle aggregation.

We used Dynamic light scattering (DLS) technique to determine the size distribution profile of small particles in suspension in order to calculate hydrodynamic radius of aspheres. For assessment of stability of colloidal dispersions we measure zeta potential of the samples. The magnitude of the zeta potential indicates the degree of electrostatic repulsion between adjacent, similarly charged particles in a dispersion. For molecules and particles that are small enough, a high zeta potential will confer stability, i.e., the solution or dispersion will resist aggregation. The method can be also used for quantification of the magnitude of the charge, which is important for studying electrohydraulic processing.

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References

- [1] J. Markhulia, V. Mikelashvili, Sh. Kekutia, L. Saneblidze, Z. Jabua, D. Daraselia, D. Jafaridze. Some physical parameters of PEG-modified magnetite nanofluids. *J. Pharm. & Appl. Chem.*, 2016, 2, 2, 33-37.
- [2] Sh. Kekutia, L. Saneblidze, V. Mikelashvili, J. Markhulia, R. Tatarashvili, D. Daraselia, D. Jafaridze. A new method of preparation of superparamagnetic nanoparticles. *Eur. Chem. Bull.*, 2015, 4, 1, 33-36.
- [3] Sh. Kekutia, L. Saneblidze, V. Sokhadze, M. Abuladze, E. Namchevadze, L. Tabatadze, G. Tvauro, V. Mikelashvili, J. Markhulia. The synthesis of PEG-modified superparamagnetic

iron oxide nanoparticles (SPIONs) and the study of their bactericidal effects on staphylococcus epidermidis. *Proc. Georg. Natl. Acad. Sci. (Ser. Chem.)*, 2017, 43, 2, 247-254.

- [4] Zh. Luo, D. Marson, Q. K. Ong, A. Loiudice, J. Kohlbrecher, A. Radulescu, A. Krause-Heuer, T. Darwish, S. Balog, R. Buonsanti, D. I. Svergun, P. Posocco, F. Stellacci. Quantitative 3D determination of self-assembled structures on nanoparticles, using small angle neutron scattering. *Nat. Commun.*, 2018, 9, 1343, 1-10.
- [5] L. Melnikova, V. I. Petrenko, M. V. Avdeev, V. M. Garamus, L. Almasy, O. I. Ivankov, L. A. Bulavin, Z. Mitroova, P. Kopcansky. Effect of iron oxide loading on magnetoferrit in structure in solution as revealed by SAXS and SANS. *Colloids & Surfaces B*, 2014, 123, 82-88.
- [6] C. Vasilescu, M. Latikka, K. D. Knudsen, V. M. Garamus, V. Socoliuc, R. Turcu, E. Tombacz, D. Susan-Resiga, R. H. A. Ras, L. Vekas. High concentration aqueous magnetic fluids: Structure, colloidal stability, magnetic and flow properties. *Soft Matter*, 2018, DOI:10.1039/c7sm02417g.

EFFECT OF γ -IRRADIATION ON STABILITY OF CYANOBACTERIA *Spirulina platensis* intact CELLS

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Spirulina platensis is one of the most promising micro algae that is used in micro algal biotechnology, because it is easy to grow and needs simple harvest and drying processes [1]. *Spirulina platensis* is rich with proteins (60 – 70 %), vitamins, minerals, and antioxidants, all of which make it highly beneficial as an antiaging, anticancer, and super-detoxifying marvel food. It is used as protein supplement in the food and pharmaceutical industry. Many characteristics of *Spirulina platensis* suggest that it may be an excellent organism for the investigation of biological interaction with ionizing irradiation.

In this work, we have studied the effect of γ -irradiation on the growth and stability of cyanobacterium *Spirulina platensis* and its constituents, using UV–VIS spectroscopy and differential scanning microcalorimetry (DSC) methods [2, 3], as well as the simultaneous effect of γ -irradiation and toxic and heavy metal ions. *Spirulina platensis* cells were exposed to γ -irradiation dose 7.2 kGy using ^{137}Cs as a gamma source at the Applied and Research Center, E. Andronikashvili Institute of Physics. The γ -irradiation effect was studied for wet, suspended and dry *Spirulina platensis* after recultivation during 14 days. The DSC and growth kinetics curves demonstrate that the irradiated cells have changed characteristics. Namely, it is shown that 7 kGy irradiation causes a decrease in metabolic heat evolution and it is 340 ± 20 cal / g of dry biomass. The C-phycocyanin heat absorption curve was shifted to higher temperatures, and a new heat absorption peak was determined at about 80 – 90°C. The nucleoprotein – genetic material – was partly damaged that was manifested in a decrease of denaturation temperature by some degrees. Addition of Cd and Pb caused heat redistribution among heat absorption peaks.

References

- [1] K. Moorhead, B. Capelli, R. G. Cysewski. *Spirulina* Nature's Super Food, 2011, Cyanotech Co.
- [2] L. Topchishvili, Sh. Barbakadze, A. Khizanishvili, G. Majagaladze, J. Monaselidze. *Biomacromolecules*, 2002, 3, 3, 415-420.
- [3] J. Monaselidze, Sh. Barbakadze, Sh. Kvirikashvili, G. Majagaladze, D. Khachidze, L. Topchishvili. *Biomacromolecules*, 2002, 3, 4, 783-786.

SMART Si SENSORS BASED ON THIN FILM NANOTRANSISTORS AS SENSITIVE ON VARIOUS EXTERNAL INFLUENCE

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In recent decades the growth rate of development and production of micro- and nanoelectronic sensors of external influences was significantly higher than that of IC's and other traditional elements and component bases. The reason is that the combination of sensorics with the automation and informatization determines the essence of modern stage of scientific and technological revolution [1]. It is quite natural that the creation of modern sensor devices and systems requires a significant improvement in the characteristics of sensors and expanding their functionality.

It is well known that at the present time microelectronic sensors mass production in most cases is based on CMOS Si technology and Si resistors as sensitive elements (SE). In this connection improvement of main Si sensor characteristics is implemented through the development of special interface IC. This leads to the complication of sensor constructions and to increase of power consumption. However, the problem can be successfully solved, if the passive SE is replaced by the active resistor controlled by the electric field (field effect sensitive element – FESE). FESE presents thin film Si transistor with double gates controlled MOS system, which channel is operating as SE. In this case it is possible to radically increase the sensitivity of sensors, to expand the range of operating temperatures, to increase resistance to any type of radiation, to reduce current consumption, to implement new design of sensors devices and microsystems, to produce multichannel and multifunctional devices with digital output signal etc. It is essential that the manufacture of FESE and corresponding sensors is based on “silicon-on-insulator” structures as a starting material and standard Si CMOS microelectronics technology processes.

The purpose of this report is to demonstrate the effectiveness of this approach for the creation of modern smart sensors of magnetic field, temperature, bioliquids, gases and other types of external influences.

Reference

- [1] I. H. Huijsing. Smart Sensor Systems: Why? Where? How? In: Smart Sensor System (Ed. by G. Meiyer), 2008, Willey & Sons, Ltd., 385 pp.

DEUTERIUM DESORPTION TEMPERATURES OF Al–Ti AND Mg–Ti COMPOSITES PREPARED BY METHOD OF ATOM-BY-ATOM COMPONENT MIXING

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Aluminium-based and magnesium-based alloys are promising in the view of present-day requirements to the metal-hydride hydrogen storage systems. Behavior of hydrogen in the aluminium-based magnesium-based alloys is of scientific and applied interest that is confirmed by many publications. However, the use of such alloys presents some difficulties because of the high hydrogen desorption temperature (550 – 600 K).

To manufacture Al–Ti composites the plasma evaporation-sputtering method was used enabling the atom-by-atom component growth. Thus, the composites with a wide range of the ratios of components were obtained. A composite was deposited on the molybdenum foils (0.2 mm thickness, 10 mm width, 250 mm length) placed between the cathode assemblies in the facility. Deuterium introduction into the samples was performed by the ion implantation method. Deuterium desorption temperature ranges and deuterium storage levels were determined by the thermal desorption spectroscopy (TDS).

A low aluminium concentration and, consequently, a high titanium concentration in the composite are demonstrated in the deuterium TDS as a single peak with a maximum temperature at 820 – 840 K as a function of the implanted deuterium dose and composite composition. A single-peak character of the deuterium TDS, observed for aluminium concentration values from 10 to 70 at. %, evidences on the homogeneity of composite structural state in this range.

As the aluminium concentration in composites increases the deuterium TDS is significantly changing and, as a result, the deuterium desorption temperature for Al₈₅Ti₁₅ composites sharply decreases ($T_m \approx 550$ K). A step-like shape of the maximum temperature curve of thermoactivated deuterium desorption, as a function of the component concentration change, evidences on the existence of two different structural states of the Al–Ti system depending on the ratio of components.

OPTICAL PROPERTIES OF Ag DOPED CdS NANOPARTICLES SYNTHESIZED BY SONOCHEMICAL METHOD

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The binary combination of cadmium element with VI groups have great interest due to unique properties. One of them is cadmium sulfide nanoparticles are widely used semiconductor with a wide range of applications. CdS nanoparticles are applicable in such areas as diodes, gas sensors, nanothermometers, solar cells, fuel cells and lithium-ion batteries (Solar Energy Laboratory, Department of Chemistry, Thiruvalluvar University, Vellore, India). The bulk CdS is a investigated n-type semiconductor with direct band gap of 2.42 eV (Department of Materials Science & Engineering, National Tsing Hua University, Hsinchu, Taiwan, Republic of China).

In this work, we prepared CdS nanoparticles by sonochemical method. $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ as cation source, Na_2S as anion source, 3-mercaptopropionic acid 99 % (MPA) as capping agent were used. MPA were used 5 %. The reaction enforce in aqueous solution permanently bubbling with nitrogen along 2 h. Gradually yellow color solution was formed. Morphology and optical properties were examined by X-ray diffractometer (XRD) and ultraviolet visible spectroscopy (UV-Vis). 0.1 M solution of Ag⁺ ion was prepared for ion exchange of obtained nanoparticles. The band gap of Ag doped CdS nanoparticles were determined by UV-Vis.

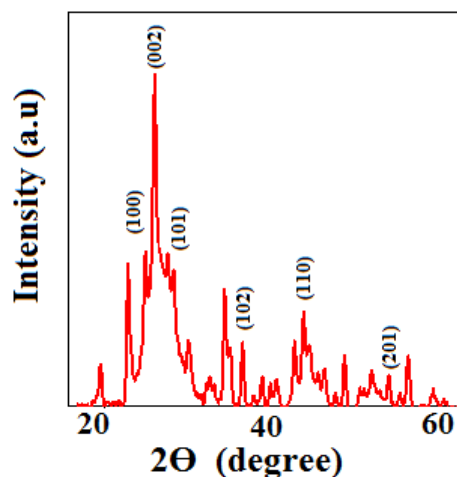


Figure 1. XRD results of CdS nanoparticles.

In **Figure 1**, the result of XRD show that the prominent peaks with 2θ values of 24.77, 25.87, 27.87, 36.03, 43.10, and 53.07 ° conform well with hexagonal wurtzite phase of CdS (JCPDS card No. 89–2944) and can be indexed according to (100), (002), (101), (102), (110), and (201) crystal planes.

The size of CdS nanoparticles were determined 28 nm by Debye–Scherer equation.

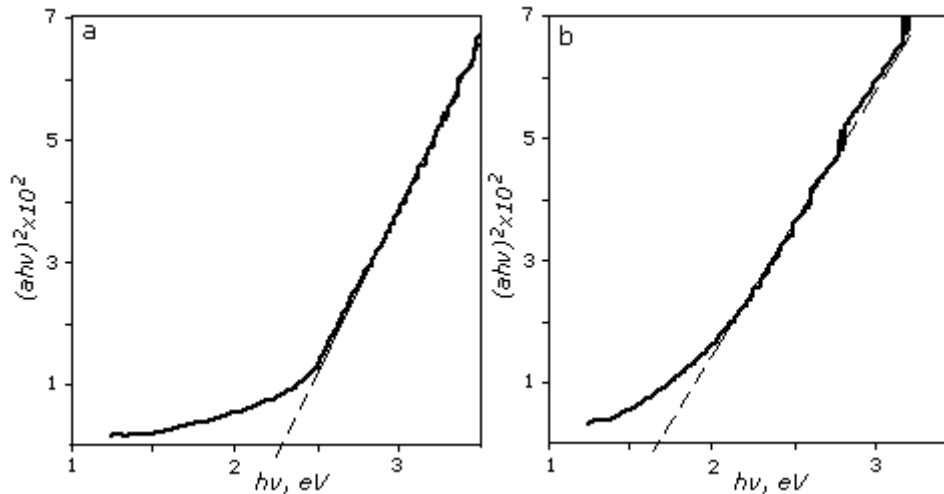


Figure 2. Band gap value of (a) CdS and (b) Ag doped CdS.

The result of UV–Vis measurements show that the band gap of cadmium sulfide nanoparticles was found 2.48 eV. The band gap value of the nanoparticles is greater than 0.6 eV from band gap value of bulk crystals (**Figure 2**). The increasing of band gap value is observed with decreasing nanoparticles size. And this explained by quantum measurement effects. In UV–Vis we can see that after ion exchange of nanoparticles with Ag⁺ ions, the band gap value of particles was decreased. This is due to with transformation of CdS nanoparticles to Ag₂S.

GROWTH OF $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ NANOPARTICLES BY LAYERED SORPTION METHOD OF IONS (SILAR METHOD)

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It is known that $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanoparticles are widely used materials in optoelectronics and electronics industries. The purpose of this work is the growth of $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanoparticles. The growth of $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanoparticles is carried out by SILAR method. The SILAR method differs from other methods of growth by its simplicity and requiring no special conditions. The experience consists of 4 stages: (i) the salts used as the source of cation are mixed with 50 mL ethylene glycol alcohol. Cd^{2+} and Zn^{2+} ions are adsorbed to the pores of the polymer matrix when the PVS polymer matrix is within 20 min of this mixture. (ii) the polymer matrix is washed in ethylene glycol alcohol to remove strangers, cation and anion residues. Ethylene glycol alcohol has been used as an intermediate washer because the PVS polymer matrix dissolves in water and in many solvents. (iii) PVS polymer matrix is inserted into a mixed container containing 50 mL of ethylene glycol alcohol and the source of anion. And a result of the reaction that occurs at this stage, $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanoparticles is formed on the polymer matrix. (iiii) The polymer matrix is still washed in ethylene glycol alcohol again.

As a source of cation: $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2x\text{H}_2\text{O}$ and $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2x\text{H}_2\text{O}$ salts have been used, and the $\text{Na}_2\text{S} \cdot 9x\text{H}_2\text{O}$ salt as the source of anion. At the experiment mole ratio of samples: a) $\text{Cd}_{0.01}\text{Zn}_{0.99}\text{S}$ and b) $\text{Cd}_{0.1}\text{Zn}_{0.9}\text{S}$. The thickness and weight of the $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ thin film were measured before and after the experiment. The thickness of thin film increased from 185 micrometer (clean PVA) to 256 μm ($\text{Cd}_{0.1}\text{Zn}_{0.9}\text{S}$) and the weight increased from 0.2721 (clean PVA) to 0.2914 g ($\text{Cd}_{0.1}\text{Zn}_{0.9}\text{S}$). The UV spectrum of the sample was measured and it was shown when the adsorption time of the ions is 20 min, the difference in the width of the prohibited zone for the 5-round sample is determined. It has been revealed that when the concentration of Cd is high, the width of the prohibited zone is extended to long waves. This indicates that in the interest rates used in practice, the $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ thin film is formed. Also the size of the particles increased with increasing number of cycles of formation. After determination band gap of sample with UV-Vis, it is possible to obtain the size of the nanoparticles. Thus, from calculation it is known that the size of nanoparticles (for $\text{Cd}_{0.1}\text{Zn}_{0.9}\text{S}$, $E_g = 3.21$ eV, $E_g^{\text{bulk}} = 3.10$ eV, $m^* = 0.00453$ g) is within 12 nm range [1]. As a result, it is possible to notice, first, that it is possible to formation of three layers of nanoparticles by the proposed methodology. And the width of the forbidden strip of formation particles depends on the chemical composition and the size of the particles.

Reerence

- [1] M. B. Muradov, G. M. Eyvazova, R. Turan, A. M. Maharramov. Effective mass and peculiarity of optical properties of cadmium sulfide nanoparticles. Optoelectron. & Adv. Mater. Rapid Commun., 2008, 2, 12, 775- 778.

ORIENTATIONAL ORDER IN N₂–Kr CONDENSED FILMS

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Molecular cryocrystals made of linear molecules have orientationally order phases. Dilution of an “orientationally neutral” rare gas atoms in a molecular crystals matrix can promote a lowering of the potential barrier, which hinders rotation of molecules in the lattice and a realization of phase transitions produced by orientational disorder [1, 2]. The degree of orientational order of the molecules in solutions could be determined from the concentration dependence of the diffracted intensity.

Observations were carried out in a standard electronograph EG–100A equipped with a helium cryostat [3]. The deposition regime was chosen in order to obtain random distributions of impurity. The samples were grown *in situ* by depositing gaseous mixtures on carbon substrate. The overall level of impurities in the source nitrogen and krypton gases did not exceed 0.01 %. The error in the lattice parameter measurements was usually 0.1 %. Observations are carried out in the temperature range from 6 to 44 K. The thickness of the deposits ranged from 100 to 300 Å. The relative error in the intensity measured did not exceed 7 %. The effect of impurity Kr atoms on the orientational ordering of N₂ molecules was studied.

The experimental dependence of the orientational diffracted intensities in N₂-based solutions was obtained. The evolution of the orientational order factor η requires the elimination of the η -independent component from the experimental concentration dependence of the intensity of superstructures lines (321). This component was determined by computation. For this purpose, the structural amplitudes for solutions with different Kr concentrations were calculated by assuming that $\eta = 1$.

The influences of composition, sample temperature, deposition temperature and subsequent subsequent heating on the orientational order factor η of the N₂ molecules in the N₂–Kr solutions were studied.

References

- [1] Eds. V. G. Mangelii, Yu. A. Freiman, M. L. Klein, A. A. Maradudin. The Physics of Cryocrystal, 1997, Woodbury, AIP Press.
- [2] B. K. Winstein. Modern Crystallography, 1979, Moscow, Nauka.
- [3] A. A. Solodovnik, N. S. Mysko–Krutik, M. I. Bagatskij. Low Temp. Phys., 2017, 43, 11, 1754.

PREPARATION GRAPHENE-CONTAINING MATRIX CERAMIC COMPOSITES USING GRAPHITE INTERCALATION COMPOUNDS

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Ceramic materials reinforced with 2D structure of graphene are characterized by high crack resistance, elasticity, electrical and thermal conductivity. Graphene injection in to the ceramic matrix is possible via several methods; among them mixing suspension of graphene and / or graphite intercalated via several chemical compounds (GIC) with powder (or precursor) of ceramic matrix. We already have received ceramic materials of Al_2O_3 , ZrO_2 , HfO_2 , B_4C , BN, Al_2O_3 –(10%) ZrO_2 , Al_2O_3 –(1%) Y_2O_3 –(0.1%) MgO containing defective graphene. Materials have been obtained using graphene oxide suspension on the matrix basis. For experiments have been used ready commercial, as well as their matrix precursor powders obtained via different methods.

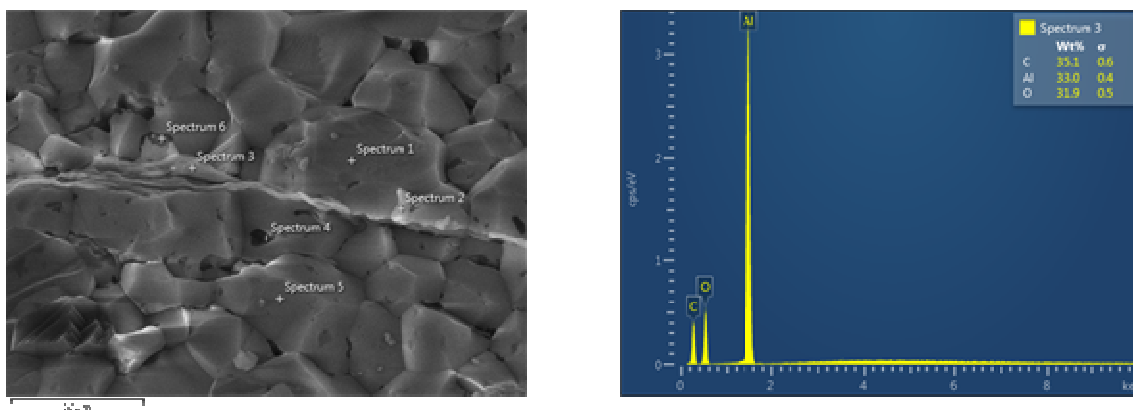


Figure 1. SEM image and EDS spectrum of Al_2O_3 graphene–ceramic composites.

Powder composites of oxide ceramics have been obtained first via adding powder of GIC in to the suspension of appropriate metals hydroxide (H_2O , DMF, GBL), and followed by ultrasonication, drying and annealing at 800 °C during 30 – 60 s. After repeated ultrasonication in to the different solvents or milling in nano miller of obtained powders has been obtained homogeneous powder of graphene-composite matrix. Consolidation of obtained powders carried out using spark-plasma sintering method at 1400 – 1900 °C for 8 – 15 min. Powders of composites and bulk samples have been investigated using XRD and SEM. **Figure 1** shows SEM and EDS images of sintered Al_2O_3 graphene-ceramic composites.

ABOUT NEW ROLE OF CLUSTERS COATED ON SURFACES OF NANOPARTICLES OF PHOTOCATALYTIC NANOPOWDERS

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At the current stage of the progress of civilization, the mankind faces major two global challenges - energy and ecology, which are closely intertwined. It is well known that, with today's rate of consumption, gas and liquid fuel supply on the Earth will soon be exhausted. Hence, it is essential to find alternative environment friendly sources of energy. The most promising direction of development of the energy of that kind is splitting of water into hydrogen and oxygen using solar energy and the use of produced hydrogen as fuel, the final product of its burning being again water, etc. [1].

Water does not dissociate by itself. For this purpose, special substances, so-called photocatalysts, are needed. Photocatalysts represent semiconductor nanopowders. Their nanoparticles create electron-hole pairs under solar light. They reach surfaces of the nanoparticles and cause water dissociation into oxygen and hydrogen using reduction-oxidation reactions. Main problem of using this reaction in a practical way is its low efficiency due to recombination of created pairs and using only UV rays in the reaction, which is the consequence of the big sized energetic gap.

A method of coating photocatalyst nanograins surfaces with various smaller sized substance clusters has been processed in E. Andronikashvili Institute of physics. As it is known, this method reduces pair recombination due to trapping electrons or holes. This method differs from other alternate methods in its low price, simplicity and, thus, it is rather competitive [2].

Coating P25 photocatalist nanograin surfaces with Ni clusters was held by this method. Optical researches showed significant growth of light absorption, which indicates on reducing electron-hole pair recombination and a increasing reaction efficiency accordingly. Interesting results were obtained in EPR researches of these nanopowders. The results showed that P25 commercial photocatalytic nanopowders and reactives, which were used to coat clusters on their surfaces don't have EPR spectras. However, after coating P25 with Ni clusters EPR spectra appeared, which had wide anisotropic singlet shape.

Obtained results indicate that clusters not only attach on photocatalytic nanoparticles while coating, they also create strong nanocomplexes with them, which can provide appearance of new energetic levels. All this indicates that clusters besides interrupting recombination, they

also implement changing photocatalyst energetic spectrum and accordingly energetic gap, which can become meaningful in any special conditions and trigger increasing the efficiency of photocatalysts.

References

- [1] K. Maeda. Photocatalytic water splitting using semiconductor particles: History and recent developments. *J. Photochem. & Photobiol. C*, 2011, 12, 4, 237.
- [2] T. Khoperia, G. Mamniashvili, M. Nadareishvili, T. Zedgenidze. Competitive nanotechnology for deposition of films and fabrication of powder-like particles. *ECS Trans.*, 2011, 35, 10, 215.

CHARACTERIZATION OF HEATER GEOMETRY FOR GAS SENSORS BASED ON SEMICONDUCTING NANOSTRUCTURES

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Semiconductor gas sensor typically consists of four main parts – substrate, heater, electrodes and layer of sensitive material [1]. The necessary power consumption, temperature uniformity and, as a result, high sensor performance can be achieved by correct choosing of heater design [2]. The material of the heater and its thickness are very important parameters for the power consuming of device [3]. And the geometry of heater element has a great effect on the temperature uniformity and temperature values. In this work four Ni heaters of different geometry were designed (**Figure 1**) and were deposited with 400 nm thickness on the silicon substrate using a thermal evaporation technique combined with a lift-off process. The study of heaters design was performed by applying different potentials to the heaters contacts. As it can be seen, the geometry has a significant influence on the working temperature values. The best results were obtained for Heater 3 and Heater 4, which were designed using the combination of the parallel and meander shapes.

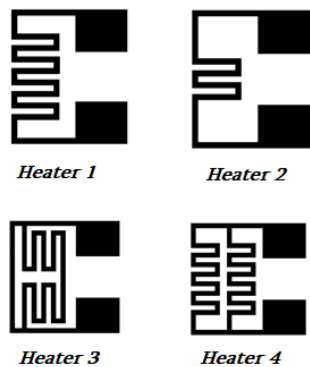


Figure 1. Geometry of heaters.

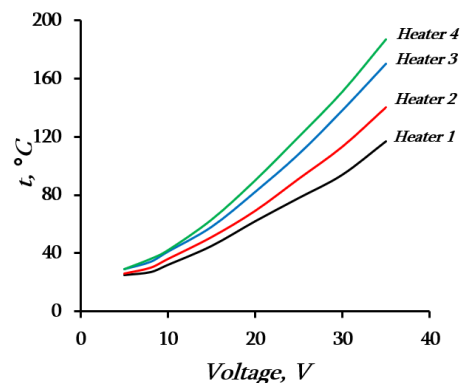


Figure 2. Temperature vs power consumption for heaters of different geometry.

References

- [1] S. Nagirnyak, T. Dontsova. In: Proc. 2017 IEEE 7th Int. Conf. Nanomater.: Appl. & Properties (NAP – 2017), 2017, 1, 333.
- [2] B. Souhir, G. Sami, C. S. Hekmet, K. Abdennaceur. Trans. Electr. & Electronic Mater., 2016, 17, 4, 189.
- [3] H. R. Khaleel, H. M. Al-Rizzo, A. I. Abbosh. Intech: Advancement in Microstrip Antennas with Recent Applications, 2013, 363.

ANTIMICROBIAL NANO-BIO-COMPOSITE ON BASIS OF SILVER IONS

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Increasing number of various infections caused by the multi-resistant microbes, spreading of mixed infections and the difficulties in struggle with them, faced medicine and pharmacy with the new challenge – seeking of natural antimicrobial agents, seeking of safe and effective biologically active substances and development of antimicrobial medicinal forms [1].

Herbal medicines, which are presented today, together with different medicinal properties has antibacterial and antiviral activities. Their effectiveness are established by the evidence based medicine. In addition, they do not cause addiction, they do not have side effects and their influence does not cause resistance on bacteria [1, 2].

Based on already conducted experiment, extract from the *Sphagnum Austinii* was chosen as a main antimicrobial agent containing silver ions. Nanoparticles were prepared using main polymers polyethylene glycol (PEG) and sodium alginate. Glucose solution and sodium hydroxide were chosen as reducing agents for formatting the spherical nanoparticles. Preparation of nanoparticles was implemented by the mixing of internal and external phases on magnetic stirrer.

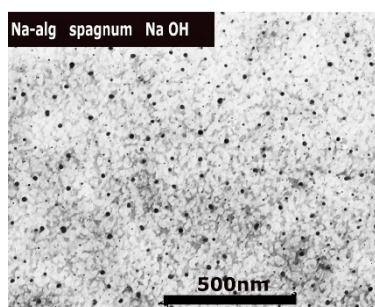


Figure 1. Sodium alginate NPs.

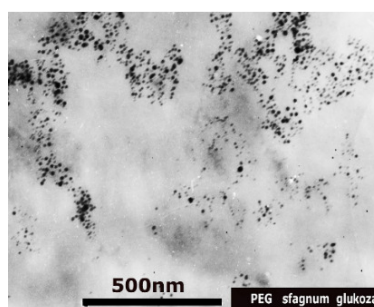


Figure 2. PEG NPs.

Standardization of the particles was conducted using electronic microscope. Results are presented in the **Figures 1 and 2**.

As it is shown, prepared nanoparticle has spherical forms and dimension varies between 40 – 50 nm. It could be established that the polymeric-matrixes polyethylene glycol (PEG) and sodium alginate are very effective carriers. Usage of reducing agents – glucose solution and sodium hydroxide causes formatting of spherical nanoparticles.

References

- [1] A. P. Shopabaeva, S. B. Khimenko, Z. B. Ospanova. Rational using of antibacterial preparats. Resistency of microorganisms. Harald Kaz. NMU, 2013, 5, 3.
- [2] M. Muradashvili, M. Metreveli, J. Jakeli, G. Meparishvili, F. Tschaidze, D. Kamadadze. Screening of Adjara seaside's dendron plant extraction *in-vitro* growth of *Ralstonia Solanacearum*. Int. J. Curr. Res., 2016, 8, 1.

FROM STATIC TO DYNAMIC NANOFRICTION – ONSET OF SLIDING

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I will discuss various theories and experimental observations related to the onset of sliding as a multiscale (from nano- to macroscale) process. The transition from stick to slip has many features similar to both phase transitions [1] and mode II crack rupture nucleation. Complex interactions govern the nucleation of frictional rupture and the transition from the stick to slip regimes, while phase transition concepts (such as the critical behavior) as well as concepts from the fracture mechanics can be applied to friction [2]. I will also discuss velocity-dependency of dry friction and effects which can be caused by such dependency [3]. In the case of very small sliding velocity, the limit of small velocity is not necessary identical to the static friction, making the phenomenon similar to the “singular limit” behavior. The laws of nanofriction vs. scaling laws of friction from macro- to nanoscale as two competing concepts will also be investigated.

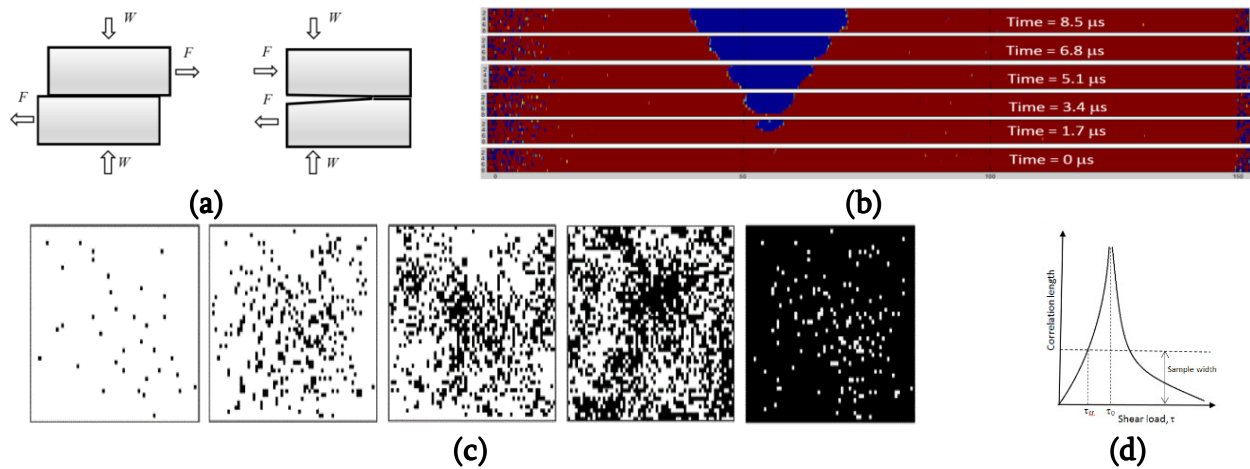


Figure 1. (a) Similarity between friction and shear mode II crack; (b) Experimental results for rupture crack initiation; (c) Typical stages of 2D percolation-type critical behavior; and (d) Typical dependency of correlation length on shear load.

References

- [1] M. Nosonovsky, V. Mortazavi. Friction-Induced Vibrations and Self-Organization: Mechanics and Non-Equilibrium Thermodynamics of Sliding Contact, 2013, CRC Press – Taylor & Francis.
- [2] I. Svetlizky, J. Fineberg. Classical shear cracks drive the onset of dry frictional motion. *Nature*, 2014, 509, 205-208.
- [3] M. Nosonovsky. Beyond the sticking point. *Mech. Eng. Mag. ASME*, 2018, 3(140), 30-35.

EFFECT OF Mg(II) ON ACCUMULATION OF
Zn(II) AND CHROMIUM IN PROTEOME OF
Arthrobacter Globiformis 151B TYPE BACTERIA

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Pollutions by *heavy metals* is a critical global environmental issue and concerns over their potential effects on human health and the environment have been raised [1]. Our studies addresses the effect of Mg(II) on the accumulation of Zn(II) and chromium in proteome of the metal resistant *Arthrobacter globiformis* 151B, isolated from the most polluted region of Georgia (Kazreti), gram-positive aerobic bacterium, involved in the microbial remediation [2].

The studies were conducted on *Arthrobacter globiformis* bacterial culture at the different growth phase after incubation in TBS broth containing 1500 µg / mL Mg at 26 °C for 16, 24, 48, 96 and 144 h. B-PER Bacterial Protein Extraction (in phosphate buffer) reagent which extracts proteins dissolved in phosphate buffer was applied to separate the dissolved and undissolved fractions. The content and concentration of Mg(II), Zn(II) and total chromium in the dissolved and undissolved layers was measured with atom absorption spectrometer.

Our result highlights active absorption of Mg(II) in proteome during first 24 h, and later after 24 h until 96 h it is slowly flushed out from the proteome and moves into the undissolved layer. However, its low concentration still remains in the proteins. The movement of Mg(II) is accompanied by increase of Zn(II) concentration in the dissolved layer, that indicates that Zn(II) can replace the same valence metal – Mg(II) in the proteins, while Mg(II) hampers accumulation of chromium in the proteins.

References

- [1] Zh. Yao, J. Li, H. Xie, C. Yu. Review on remediation technologies of soil contaminated by heavy metals. *Procedia Environm. Sci.*, 2012, 16, 722- 729.
- [2] N. Y. Tsibakhashvili, T. L. Kalabegishvili, A. N. Rcheulishvili, H.-Y. Holman. Effect of Zn(II) on the reduction and accumulation of Cr(VI) by *Arthrobacter* species. *J. Ind. Microbiol.*, 2011, 38, 11, 1803-1808.

MODEL OF DISORDERED REGIONS IN IRRADIATED SILICON

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New model of disordered regions in irradiated single-crystalline silicon is developed based on measurements of electrophysical parameters temperature-dependences in n-Si:P and p-Si:B samples irradiated at room temperature with high-energy protons and electrons, respectively, and isochronously annealed at various temperatures.

Disordered regions are imagined as relatively high-conductive inclusions with increased concentration of radiation defects separated by Ohmic interfaces with relatively low-conductive matrix. Initially, these regions are electrically neutral, but depending on the annealing mode the constituting radiation defects can change their charge-states.

COBALT-CONTAINING NANOCOMPOSITES FOR CATALYTIC HYDROGENATION OF QUINOLINE

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Catalytic hydrogenation processes are widely used in modern organic chemistry for synthesis of active pharmaceutical ingredients, biologically-active compounds for agrochemistry, etc. Such reactions are usually carried out with catalysts, based on platinum group metals (Pt, Pd, Rh), which are quite expensive. Search of active catalysts containing only 3d metals for large-scale hydrogenation processes is an important task [1].

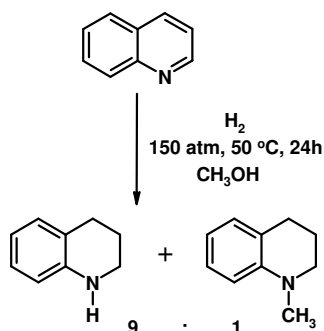


Figure 1. Reaction scheme. Products ratio is indicated for one of the samples.

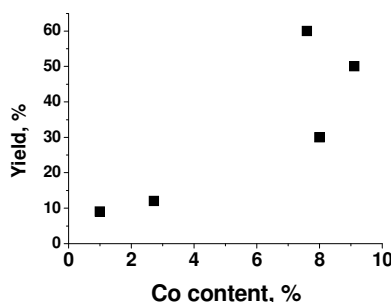


Figure 2. Yields of 1,2,3,4-tetrahydroquinoline vs. Co content in samples.

In this work catalytic activity of the Co-containing nanocomposites based on carbon (or graphene oxide) and polyindole (PIn) or poly-*m*-phenylenediamine (PmPDA) in reaction of quinoline hydrogenation was studied (**Figure 1**). The yield of 1,2,3,4-tetrahydroquinoline generally grew with increase of Co content (**Figure 2**), but also depended on the structure of the composite. Addition of PmPDA to the composite instead of PIn resulted in 2-fold increase of its catalytic activity at similar Co content (**Figure 2**). From the other hand, catalytic activity of the composites which containing PmPDA or Pin, was higher, compared to the ones, based on solely carbon or N-doped carbon carrier.

Reference

- [1] R. V. Jagadeesh, T. Stemmler, A.-E. Surkus, M. Bauer, M.-M. Pohl, J. Radnik, K. Junge, H. Junge, A. Bruckner, M. Beller. *Nature Protocols*, 2015, 10, 916.

ABRUPT REDUCTION IN CONCENTRATION OF CURRENT CARRIERS IN DOPED IV–VI SEMICONDUCTORS UNDER “NEGATIVE” PRESSURE

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Narrow-bandgap IV–VI semiconductors widely used in IR optoelectronics. In particular, based on these semiconductors, tunable lasers and photodetectors are designed. With doping these semiconductors with variable-valence impurities (Cr, In, Yb, and others) the conditions for reducing the concentration of current carriers due to mutual compensation of electrically active nonstoichiometric defects and impurity states having opposite signs. To observe such an effect in the compositions of this kind, including the ones with wider band gaps, it was suggested to use “negative” pressure, when the layers are grown on the substrates with a larger lattice constant. Under such conditions, the band gap width increases, and this process enhances with manifestation of variations in elastic constants. These effects reveal effectively at nanothickness of the layers.

The following heterostructures were suggested and fabricated: PbSnSe/PbTe, PbSnTe/EuTe and PbSnTe/BaTe. Under “negative” pressure ~ 10 kbar and at 77 K, the band gap width was 0.4 eV, and, when doping with Cr and In, the concentration of current carriers decreased below 10^{10} cm^{-3} (in the unstrained layers it was equal to 10^{18} cm^{-3}). The state of the level, in particular, of In is lower than the conduction band edge and made up ~ 0.1 eV. The typical values of the rate of variation in the impurity level state with changes in the composition were

$$\frac{dE_i}{dx} = 5 - 7 \text{ meV} / \%,$$

the band gap width and the state of the impurity level were changed with temperature as

$$\frac{dE_g}{dT} = 4 \cdot 10^{-4} \text{ eV} / \text{K}$$

and

$$\frac{dE_i}{dT} = -3 \cdot 10^{-4} \text{ eV} / \text{K},$$

respectively.

With such significant reduction in the concentration of current carriers in the layers, the dielectric state is formed, and the Fermi level is stabilized in the vicinity of the impurity level. Based on the materials of this type, high-sensitive photodetectors for the spectral range of $3 - 20 \mu\text{m}$ are designed.

References

- [1] A. M. Pashaev, O. I. Davarashvili, V. A. Aliyev, M. I. Enukashvili, V. P. Zlomanov. Regular connection between simultaneous stabilization of the Fermi level and transformation of the elastic properties of IV–VI semiconductors with their conversion into the dielectric state. *Int. Acad. Auth. Sci. Discoveries*, 2008, Moscow, Scientific Discovery No. 340.
- [2] A. Pashaev, O. Davarashvili, M. Enukashvili, R. Gulyaev, V. Zlomanov. Unrelaxed state in epitaxial heterostructures based on lead selenide. *J. Mod. Phys.*, 2012, 3, 6, 502-510.

FEATURES OF SYNTHESIS OF GOLD NANOPARTICLES USING REAGENTS OF GREEN CHEMISTRY

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The widespread use of nanoparticles is due to their unique properties. Currently, to obtain nanoparticles, various physical and chemical methods are used. However, often, these methods are expensive and time-consuming, and the use of toxic reagents is associated with a danger to the environment, living organisms and operating personnel. In this regard, an alternative approach to the synthesis of nanoparticles using green chemistry reagents is being actively developed. This approach also contributes to easier control over the size and shape of nanoparticles. Due to their unique physicochemical properties, gold nanoparticles attract particular attention of researchers and are widely used in medicine, biotechnology, fiber optics, in the creation of various sensors, etc.

In the present work, the synthesis of gold nanoparticles from chloroauric acid HAuCl_4 with the help of sodium citrate and tannin is considered. Sodium citrate $\text{Na}_3\text{C}_5\text{H}_5\text{O}_7$ is non-toxic and is widely used in the food industry and medicine. Tannin is an amorphous phytogenous powder of astringent taste with a slight peculiar smell, well soluble in water. It is widely used in medicine, in the technology of various drinks and as a coloring agent.

The studied solution was prepared at room temperature (0.5 % tannin and 1 % sodium citrate) with constant stirring, then added to a 0.01 % solution of HAuCl_4 and adjusted to pH 8.2 using sodium carbonate. The resulting solution acquired a ruby-red color, indicating the appearance of gold nanoparticles. Optical absorption spectra were recorded at room temperature on a UV Spectrometer "SINTRA10e" spectrometer. The surface plasmon resonance spectra under study had a maximum at 553 nm. The analysis of the obtained nanoparticles was performed using a Jem-100Sx transmission electron microscope. The formed gold nanoparticles were of spheroid and ellipsoidal form, as well as in the form of nanotriangles. The sizes of the obtained nanoparticles were mainly within the range from 15 to 35 nm. In addition to these particles, a small amount of particles > 35 nm in size was detected. It should also be noted that the solution was processed in a microwave furnace. The microwave exposure provided a very fast and uniform heating of the solution and contributed to obtaining nanoparticles of equal shape and smaller size. Microwave treatment of the solution was carried out for ten minutes at a power of 600 W. A shift of the absorption maximum in the surface plasmon resonance spectrum towards short waves (537 nm) caused by the process of fragmentation of gold nanoparticles in solution was also observed. Histograms were constructed for the distribution of gold nanoparticles in size before and after microwave exposure. Studies have shown that the tested method is inexpensive, requires relatively simple technical facilities, has good reproducibility, provides effective control over the size and shape of nanoparticles and has a good prospect for application in the biomedical field.

PREPARATION OF SILVER NANOPARTICLES FROM SILVER NITRATE USING CINNAMON

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Silver nanoparticles have unique optical properties due to surface plasmon resonance. They have a developed surface, are catalytically active, have excellent antibacterial properties. Due to this combination of properties, they are widely used to create electronic and optical sensors. Colloidal solutions and substances with silver nanoparticles are promising in such areas as medicine, production of hygiene items, sportswear and creation of antibacterial drugs.

Silver nanoparticles can be obtained by various methods among which is a rapidly developing synthesis using plant extracts. The advantages of this method are shorter synthesis time, low cost, safety for the environment and maintenance personnel.

In the present work, the preparation of silver nanoparticles from silver nitrate with the use of ground cinnamon, which serves as a reducing agent for silver ions, is considered. For the synthesis of silver nanoparticles, a AgNO_3 solution with concentration of 10^{-2} M was used. Distilled water was used to prepare the solution. A solution of ground cinnamon was carefully stirred and, after filtration, mixed with a solution of silver nitrate and treated using a magnetic stirrer. After further heating in a water bath at 80 °C for 30 min, the color of the solution turned brown-red, which indicated the appearance of nanoparticles.

Optical absorption spectra were recorded on a UV Spectrometer SINTRA-10e. Surface plasmon resonance spectra had a maximum at 440 nm. The geometric shapes and sizes of nanoparticles were studied using a Jem-100Sx transmission electron microscope. Spheroid, ellipsoid and rectangular nanoparticles were synthesized. The sizes of these nanoparticles were in the range of 5 – 50 nm. Histograms for the distribution of nanoparticles in size were constructed. A mechanism of formation of nanoparticles obtained using the solution of plant extracts was studied.

The method allows one to obtain silver nanoparticles with controlled parameters and is promising for large-scale applications.

SYNTHESIS OF COPPER NANOPARTICLES USING COPPER SULFATE AND RED WINE

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Currently, copper nanoparticles are of increased interest, which is associated with their specific properties. Copper-based nanoscale materials are widely used in chemical sensors to create catalysts and nanocomposites for medical purposes.

One of the chemical methods for producing copper nanoparticles is a synthesis of copper salts with borohydride and hydrosin. Copper nanoparticles synthesized in an aqueous medium using borohydride have low stability, are contaminated with boron and are easily oxidized by atmospheric oxygen. Therefore, the addition of surfactants is required to prevent nanoparticles from oxidation and aggregation.

Hydrosine has a high reducing stability, however, in this case, copper forms sparingly soluble hydroxides, which reduces its reactivity. At the same time, these substances are highly toxic. An alternative method is the use of green chemistry reagents.

In the present work, the formation of copper nanoparticles from copper sulphate with the help of Saperavi wine is considered. Wine was used as a reducing agent and a stabilizing reagent. Synthesis was carried out at room temperature. Distilled water was used to prepare a solution of copper sulfate (10^{-2} M). Then red wine was added to this solution and mixed thoroughly. Optical absorption spectra were recorded on a UV "SINTRA-10c" spectrometer. The spectra had a surface plasmon resonance with a maximum at 540 nm. The analysis of the synthesized nanoparticles was carried out using a Jem-100Sx transmission electron microscope. The resulting copper nanoparticles were of spheroid, ellipsoid, and triangular form. Histograms were constructed for the distribution of copper nanoparticles in size.

The studies have shown that the tested method has good reproducibility, is relatively simple, inexpensive and is very promising for application in biomedicine and other fields.

STRUCTURAL STABILITY OF FERROFLUIDS IN BULK AND AT INTERFACES BY NEUTRON SCATTERING

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Magnetic fluids or ferrofluids (FFs) are fine liquid dispersions of magnetic nanoparticles (MNPs) (characteristic size ~ 10 nm) covered with surfactants for preventing their coagulation in different conditions. The understanding of mechanisms of ferrofluids stability is an important factor in the synthesis of highly stable magnetic colloids with defined properties. Diagnostic of aggregation and determination of the aggregation regimes and their control in biocompatible magnetic fluids are necessary for their development in biomedical applications. Behavior of magnetic nanoparticles in bulk and at interfaces can be very different due to specific adsorption properties, which should be considered in a variety of applications. An open question is the possible differences in the FF stability in bulk and at interfaces.

Neutron scattering is powerful technique for structure diagnostic of various objects within length scale 1 – 100 nm in bulk (small-angle scattering method) and at interface (neutron reflectometry). Various types of magnetic fluids on non-polar organic solvents and on water were considered [1]. Diagnostic of aggregation and determination of the aggregation regimes were done for water-based FFs. Also the microstructure of non-polar ferrofluids with excess of surfactant and inter-particles interaction were investigated by SANS.

It was observed that the structural organization of nanoparticles at interface depends on the MNPs concentration in ferrofluids, as well as on the structural organization of MNPs in bulk. Also, the impact of the stabilization type of FFs together with the kind of magnetic components was investigated. The influence of gravity and external magnetic field on the adsorption properties of magnetic particles and their behaviour at interface was considered including free surfaces (air/FFs). Mono- and multi-layered structures of ferrofluids at interfaces were studied. The possibility of anchoring MNP from FFs on substrates by external magnetic fields was discussed. It was obtained that along with the structural stability in bulk the considered MFs are characterized by the interface stability as well.

Reference

- [1] V. I. Petrenko, A. V. Nagornyi, I. V. Gapon, L. Vekas, V. M. Garamus, L. Almasy, A. V. Feoktystov, M. V. Avdeev. Ch. 10: Magnetic fluids: structural aspects by scattering techniques. In: Modern Problems of Molecular Physics. Sel. Rev. Springer Proc. Phys. (Eds. L. Bulavin, A. Chalyi), 2018, Springer, 205-229.

ECOFRIENDLY SYNTHESIS OF GOLD NANOPARTICLES USING PHYTOEXTRACTS

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Increasing interest to nanotechnology leads to the revision of existing and developing methods for the nanoparticles synthesis. To date there are several different approaches to synthesis of nanoparticles. Biological methods of nanoparticles synthesis (using microorganisms, cell culture, plant tissue or phytoextracts) were proposed as possible environmentally safe methods which are alternatives to existing chemical and physical methods of nanoparticle synthesis [1, 2]. While microorganisms such as bacteria, actinomycetes, and fungi have long been used in synthesis of metal nanoparticles, the use of plants in similar nanoparticle synthesis techniques is rapidly developing [3]. Results on the reduction potential of phytochemicals present in tea to reduce gold salt (NaAuCl_4) to the highly homogenous gold nanoparticles are described. Respective phytoextracts derived from the mixture of *Thea sinensis* var. *sinensis* + *Thea sinensis* var. *assamica* (green tea) leaves. The sloping peak absorption of the phytoextract and gold salt solution after reaction at the wavelength range 530 – 550 nm corresponded to the absorption of gold nanoparticles. Obtained nanoparticles were purified after reaction from phytoextract excess by centrifugation and then they were studied by Raman and FTIR spectroscopy as well as by AFM. The size of gold nanoparticles was in a range about 3 – 10 nm. The tea-generated gold nanoparticles have demonstrated respective stability under experimental conditions. We consider this truly biogenic, green nanotechnological process as the way opening excellent opportunities for further applications of obtained gold nanoparticles in molecular imaging and therapy.

References

- [1] D. P. Debecker, C. Faure, M.-E. Meyre, A. Derre, E. M. Gaigneaux. *Small*, 2008, 4, 1806.
- [2] A. Ahmad, P. Mukherjee, D. Mandal, S. Senapati, M. I. Khan, R. Kumar, M. Sastry. *J. Am. Chem. Soc.*, 2002, 124, 12108.
- [3] S. Shankar, A. Rai, A. Ahmad, M. Sastry. *J. Colloid & Interface Sci.*, 2004, 275, 496.

INFLUENCE OF Na ON PROCESS OF Zn ASSIMILATION BY *Arthrobacter globiformis* 151B TYPE BACTERIA

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Arthrobacter globiformis 151B type bacteria are able to assimilate different chemical elements, e.g. Cr, Zn, Cu etc. from the environments [1]. The ions of chemical elements that got into bacteria take part in different biochemical processes. It is supposed that some microelements (Na, K, Mg) have an influence on the process of assimilation of Cr, Cu, and Zn [2] in bacteria.

The influence of Na on assimilation of Zn in *Arthrobacter globiformis* 151B type bacteria has been studied. The solution of Zn was introduced into “TSB” nutrient medium and its concentration in the medium made 5 µkg / mL. At the same time, Na solution (NaCl) of different concentrations was introduced as well: 1.5 mg / mL into 5 flasks, 4.5 mg / mL into 5 flasks and 7.5 mg / mL into 5 flasks; The bacteria were growing during 17 and 24 h, nd 2, 4, and 6 days. The concentration of Zn in the obtained samples was measured by the method of atom absorption spectrometry. The results are shown in the **Figure 1**.

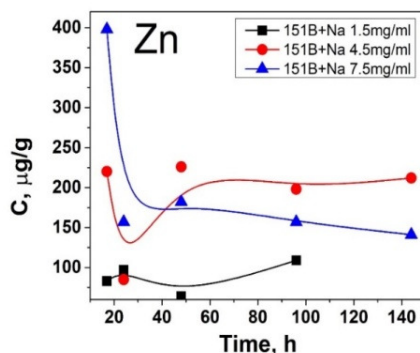


Figure 1. Dependence of Zn concentration on time of growing in *Arthrobacter globiformis* 151B type bacteria.

From the obtained results we can suppose that in the case of increased dose of Na concentration in the nutrient medium the assimilation of Zn in *Arthrobacter globiformis* 151B type bacteria is increased.

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References

- [1] R. Choudhury, S. Srivastava. Zinc resistance mechanism in bacteria. Curr. Sci., 2001, 81, 768-775.
- [2] N. Y. Tsibakhashvili, L. M. Mosulishvili, T. L. Kalabegishvili, E. I. Kirkesali, I. G. Murusidze, S. M. Kerkenjia, M. V. Frontasieva, H. Y. Holman.. Biotechnology of Cr(VI) transformation into Cr(III) complexes. J. Radioanal. Nucl. Chem., 2008, 278, 565-569.

INFLUENCE OF SODIUM ON PROCESS OF ASSIMILATION OF CHROMIUM BY *Arthrobacter globiformis* 151B TYPE BACTERIA

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Arthrobacter globiformis 151B type bacteria assimilate intensively Cr(VI) from the environment, convert it into Cr(III) and accumulate it [1]. The existence of Zn(II) in bacteria nutrient medium strongly increases the accumulation of chromium from the environment and the intensity of its conversion into Cr(III) [2]. It is expected that the process of assimilation of Cr(VI) is influenced by the other elements widely spread in nature.

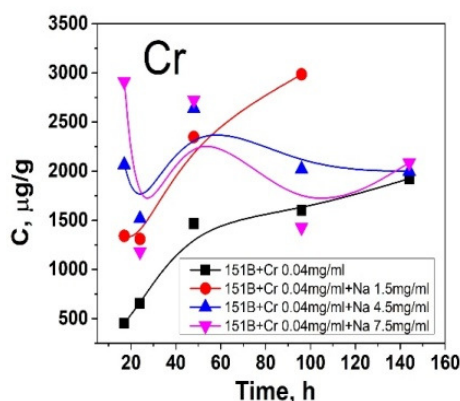


Figure 1. Dependence of concentration of Cr in *Arthrobacter globiformis* 151B type bacteria on time of bacteria growing.

The influence of Na on the process of Cr assimilation has been studied. Cr(VI) solution the concentration of which in the nutrient medium made 40 µg / mL was introduced into “TSB” nutrient medium. At the same time, Na solution was introduced into different flasks: 1.5 mg / mL into 5 flasks, 4.5 mg / mL into 5 flasks, and 7.5 mg / mL into 5 flasks. Bacteria were

growing during 17 and 24 h, and 2, 4 and 6 days. The analysis of the obtained samples for the content of Cr was carried out by atom absorption spectrometer. The results are shown in the **Figure 1**. As it is seen from the obtained results, the existence of sodium in the nutrient medium favors the assimilation of chromium by *Arthrobacter globiformis* 151B type bacteria.

The work is performed within the frames of Grant STCU 6316/SRNSF STCU 2016/09.

References

- [1] T. Kalabegishvili, et al. Environ. Sci. & Technol., 2003, 37, 20, 4678-4684.
- [2] N. Tsibakhashvili, et al. Ind. Microbiol. & Biotechnol., 2011, 38, 11, 1803-1808.

BIOCHIP APPLICATION FOR CONTROL OF MICROBIAL COMMUNITY WITH HEAVY METAL REMEDIATION POTENTIAL

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Bacteria are regarded as the most effective in the detoxification of heavy metals, being environmental compatible. The intensive study of contaminated area has revealed the selective metallophilic properties of bacteria. Since the effect of some heavy metals on the soil leads to the activation of specific forms of microorganisms, interacting with certain metals and thereby surviving in conditions of soil contamination, we have evaluated composition of microbial communities with the heavy metals bioremediation potential, using low-density biochip. Once there are some restrictions on the microorganisms' introduction in the environment, it is important to establish the bioremediation potential of native species from a particular location for their further use in the bioaugmentation process.

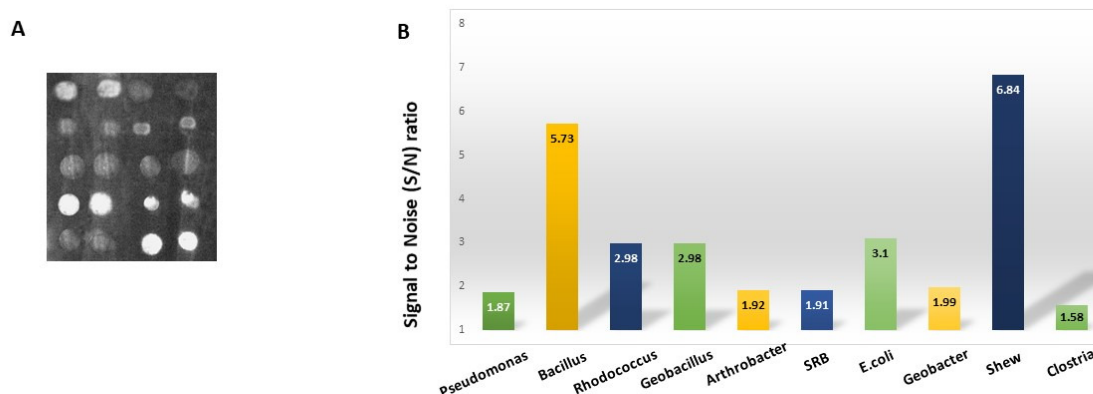


Figure 1. DNA of soil was amplified and hybridized with biochip. Panels (A) represents hybridization image; Panels (B) shows hybridization signal, presenting as signal to noise ratio.

The biochip identifies the following bacterial consortium *Rhodococcus*, *Bacillus*, *E. coli*, *Pseudomonas*, *Shewanella*, *Geobacter*, *Arthrobacter*, *Geobacillus*, *Clostridia* spp. and sulfatereducing bacteria (SRB). As it follows from **Figure 1** the studied non-contaminated soil contains all of these species; however, the *Bacillus* and *Shewanella* spp. dominate. Both of them are characterized by high remediation potential and could be used in the bioremediation and bioaugmentation processes.

EFFECT OF CONCENTRATED LIGHT ON MIXTURE OF BORON AND ALUMINUM POWDERS TRANSFORMATION IN FLOW OF NITROGEN

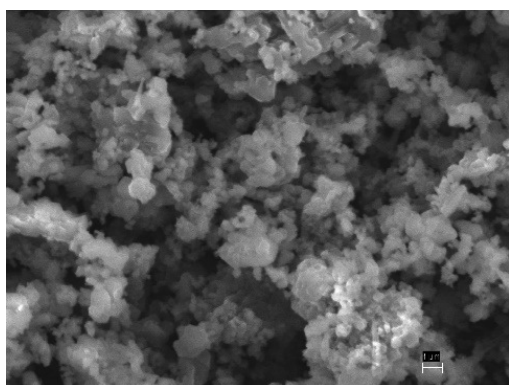
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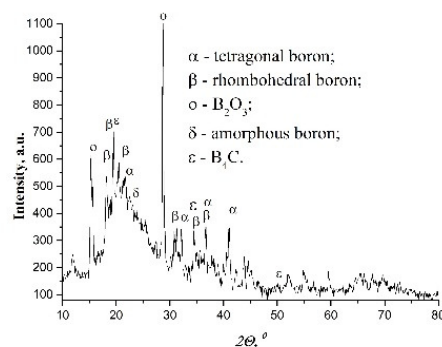
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Transformation of boron (B) powder and 25 wt. % aluminum (Al) powdered additive was considered. Heating of initial powders was carried out in a xenon high-flux optical furnace in a nitrogen flow at the temperatures 1000 – 1400 °C. It was demonstrated that addition of aluminum results in formation of H_3BO_3 , amorphized BN and AlB_{12} (**Figure 1**).

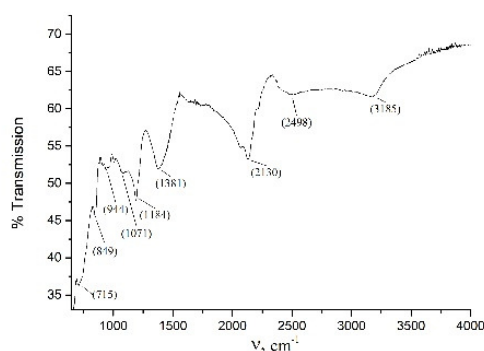


(a)



(b)

Figure 1. SEM image (a), XRD pattern (b), and FTIR spectra of initial boron powder.



(c)

The absence of components of aluminum oxides in produced composite specifies boron as a strong getter. Presence of AlB_{12} changes FTIR and Raman spectra of BN in the obtained composite nanostructures.

SYNTHESIS OF NANOSTRUCTURES UNDER EFFECT OF CONCENTRATED LIGHT AND RESEARCH PROBLEMS FOR THEIR PROPERTIES

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In this study, results of synthesis of the boron nitride (BN) and BN based composite nanopowders under effect of concentrated light are considered. Composite nanopowders based on BN were prepared by incorporation of 25 wt.% metal additives to boron powder by mixing. Heating of precursors was performed in a xenon high-flux optical furnace in a nitrogen flow at the temperatures 1000 – 1400 °C. The effect of metals additives on the microstructural behavior of the developed BN composites was studied in comparison with pure BN using the structure-property correlation. Infrared and Raman spectroscopy along with optical microscopy was *performed*. BN and BN composite nanoparticles were characterized by XRD and TEM measurements. Experimental results on the concentrated light heating of boron and boron incorporated of 25 wt. % metal additives nitride are interpreted.

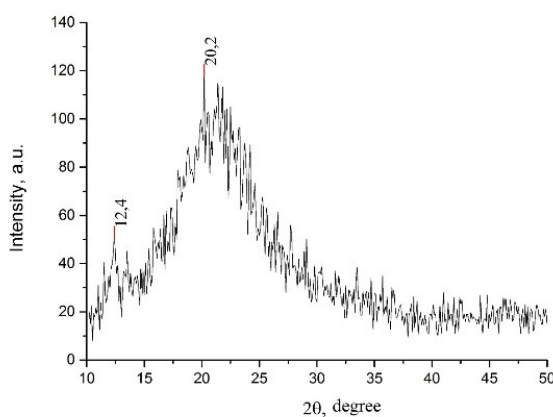


Figure 1. XRD pattern of amorphized BN.

Transformation of black boron powder into a white or gray powder depending on metal content was observed indicating the presence of BN. XRD studies confirmed the formation of amorphized BN on the surface of boron powder under effect of concentrated light (**Figure 1**). In some cases, the incorporation of metals results in appearance of a number of metal borides, shifting a main peak of amorphized BN in XRD pattern, disappearing and shifting some peaks of infrared and Raman spectroscopy.

MODIFYING THE PROPERTIES OF CEMENT AT ADDITION OF METAKAOLIN RECEIVED BY HEAT TREATMENT OF SHALES

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In recent years, there is a great popularity in the world use of metakaolin as an effective pozzolanic additive to cement. The addition of Metakaolin (due to the high specific surface area – up to 13000 cm² / g) allows to increase the density, water resistance and strength of cement, thus making it possible to reduce the consumption of clinker – an energy-intensive and expensive product of the cement industry. Metakaolin is obtained by heat treatment of kaolin clays, the deposits of which are strictly limited. Therefore being developed to study the possibility of obtaining metakaolin from regular polymer clay that would be much cheaper and would make available this material.

For our experiments the alluvium of clay shales from the banks of the river Duruji, collapsing rock of the Caucasus range formed as a result of mud-mud flows, was used. Clay shales were studied by chemical, petrographic, X-ray phase and differential thermal analysis, which have revealed a tendency of phase transformations at their heating in the range of temperatures from 20 to 1000 °C.

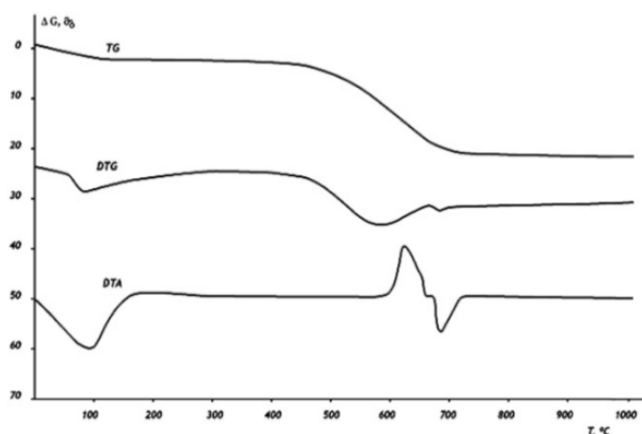


Figure 1. The DTA pattern of shales.

Table 1. Physical-mechanical properties of cements.

Cement composition, wt. %	Compression Strength after 28 days, MPa	Changes in cement activity, %
Clinker – 95 Gypsum – 5	35.6	–
Clinker – 85 Shale – 10 Gypsum – 5	37.9	+ 6.5
Clinker – 75 Shale – 20 Gypsum – 5	33.5	– 5.9

The temperature range from 680 to 750 °C endothermic effect, which is associated with the destruction of the crystal lattice of clay minerals and their transition to the active amorphous form – metakaolin, was revealed on the DTA curves (**Figure 1**).

The mode of heat treatment of clay shale is developed, at which the maximum presence of metakaolin is provided. To determine the pozzolanic properties of calcined clay shale, cements were made using the ASTM C 311–05 standard test methods for sampling and testing fly ash or natural pozzolans for use in portland-cement concrete method. The test results are given in **Table 1**.

The obtained results enable to conclude that the thermally processed shale, which contains a number of metakaolin, can be a spectacular pozzolanic additive for cement.

RAPID SYNTHESIS OF FUNCTIONAL OXIDE MATERIALS BY LIGHT IRRADIATION

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Most of the technologically important oxide materials are usually obtained through solid-state reactions. This implies long-term (tens of hours) heating of reactants in powder form at high temperatures in a furnace, a highly time- and energy-consuming process. Moreover, the long-term high-temperature synthesis may result in deviation from the original stoichiometry and other unwanted side effects. Therefore, there is a significant worldwide effort to develop technologies to considerably reduce the solid-state reaction temperature and time.

We report a novel kind of oxide synthesis, which involves the irradiation of the mixture of precursors with light in a broad spectral range, from infrared to ultraviolet, and sufficient intensity to initiate the solid-state reaction between the reagents contained in the powder mixture. By using this method, we could synthesize different superconducting and magnetic oxides. It was demonstrated that light irradiation leads to a dramatic increase of the solid state reaction speed and a lowering of the reaction temperature. The rate of the resulting reaction exceeds conventional thermal solid-state reaction rates by about two-three orders of magnitude. The photo-stimulated solid-state reaction (PSSR) method is confirmed to be quite general and opens up the possibility of fast synthesis of a wide range of technologically important bulk and thin-film oxide materials.

COMBINATION OF MECHANICAL ALLOYING AND SPARK PLASMA SINTERING TECHNIQUES AS NOVEL APPROACH FOR CONSOLIDATION OF Cu-BASED NANOSTRUCTURED PSEUDO ALLOYS

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Due to excellent combination of high mechanical, electrical and thermophysical properties Cu-based matrix composites (also called pseudo alloys) from immiscible metals have been of current interest. They find a variety of applications including heat-sink elements in microelectronic devices, electrical contacts, as well as plasmatron nozzles for rocket engines.

Difficulties in production of high quality pseudo-alloys are related to low mutual solubility of metals, high difference between their melting points and densities, and high wetting angle. And it cannot be overcome completely through the conventional melting and casting methods.

In the present study, a combination of high-energy ball milling (HEBM) and spark plasma sintering (SPS) methods has been shown to be suitable for the production of highly dense Cu–Cr–W nanostructured bulk materials.

Mechanical treatment of Cu–Cr–W powder mixtures was carried out in an Activator–2S planetary mill (steel balls 7 – 9 mm, ball mill ratio 20 : 1, τ = 30 – 150 min), while sintering, in a Labox 650 (Sinter Land, Japanese) System in a vacuum at different temperatures (600 – 900 °C) under pressure (50 MPa). Synthesized alloys were characterized by XRD, SEM, and EDS.

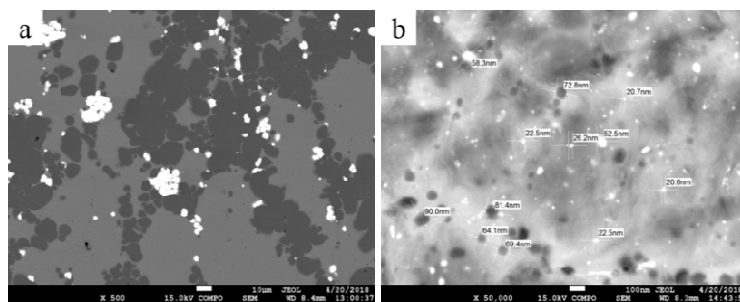


Figure 1. SEM images of (a) starting and (b) activated Cu–Cr–W composite SPS-consolidated at 800 °C for τ = 150 min; in (a): dark grey Cr, white W, grey Cu; in (b): white W, dark grey Cr, rest Cu matrix.

The results in **Figure 1** suggest that the structure of the Cu–Cr–W composite formed at the stage of HEBM is retained after SPS consolidation. Specific conductivity of our composite is above 25 % of International Annealed Copper Standard ($1.72 \mu\Omega \text{ cm}$), which is quite tolerable for electrocontact materials. The combined use of HEBM and SPS looks rather promising as a route to fabrication of consolidated nanocrystalline psuedoalloy-based Cu–Cr–W composites.

PALS STUDY OF RARE-EARTH DOPED Se-BASED GLASSES

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Rare-earth (RE) doped chalcogenide glasses (ChG) attract great attention in modern materials science community as versatile device media for a variety of active applications in mid-IR optics including fiber-optics amplifiers and IR lasers. However, this sphere of chalcogenide photonics has still being highly disputable now because of insufficient knowledge on the nature of RE-activated functionality in covalent-saturated ChG networks.

In this work, the method of positron annihilation lifetime (PAL) spectroscopy, which is known as advanced instrumentation tool efficiently exploring nanospace at atomistic and sub-atomistic length-scales, was applied to study the mechanism of RE-doping in Se-based ChG.

The most efficient positron traps in parent (As/Sb)₂Se₃ glass are shown can be imaged as free-volume voids formed within cycle-type arrangement of directly corner-sharing trigonal (As/Sb)Se_{3/2} pyramids, composed of atomic-accessible geometrical holes arrested by surrounding atomic-inaccessible Se-based bond-free solid angles (**Figure 1**).

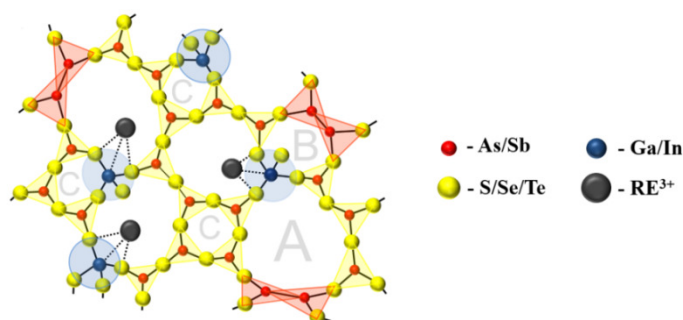


Figure 1. Sketch of plane projection of void structure of (As/Sb)₂Se₃ built of corner-sharing (As/Sb)Se_{3/2} pyramids showing character cycle-type arrangement with free-volume voids in RE-modified glass.

Effect of RE doping (500 wppm of Pr³⁺) in As–Se-based glass is explained in terms of competitive contribution of changed occupancy sites available for rare-earth ions and annihilating positrons being trapped in Ga-modified network. Under doping, the Pr³⁺ ions are stabilized due to Pr³⁺–Se–Ga linkages, thus eliminating neighboring void as potential positron trapping sites. Effect of rare-earth doping in the studied glass results in notably reduced positron trapping rate in free-volume voids, originated from their decreased content and rather slightly altered volume.

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POTENTIAL HAZARDOUS INFLUENCE OF NANOSIZED ADMIXTURES USED FOR PRODUCTION OF CEMENT-BASED COMPOSITES ON ENVIRONMENT

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The intensive development of nanotechnology, manifested by the huge amount of available nanoproducts, allows the production of modern composites in many fields of science. One of these areas that has benefited in recent years from the development of nanotechnology, is construction sector, including the technology of cementitious composites (e.g. cement mortars and concrete). The production scale and the wide application range of nanomaterials have made the presence of these structures in the environment unavoidable, where the effect can be the release to the natural environment. It is of a great importance in the case of cementitious composites, due to the constant exposition of building elements to the environment. These conditions may result in the release of nanomaterials into water, soil and air, which may pose a threat to humans and the environment.

In our study, Al₂O₃, CuO, Fe₃O₄, and ZnO nanoparticles (commonly used as admixtures to cement-based composites) were used and tested on reference strains of *Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus aureus* and *Candida albicans*. Nanomaterials were used according the standard procedures used in the preparation of cementitious composites. The morphology and viability of cells were tested with microscopy, spectrophotometry, and culture methods. The results revealed that nanoparticles may decrease their antimicrobial efficiency, possibly due to the aggregation process. Even though the studied particles were toxic to subject microorganisms in acute tests, the populations were able to re-grow when co-incubated with the nanoparticles in the liquid medium. Furthermore, we found a considerable diversity in the reaction of tested strains to nanoparticles, even between four different strains of *Escherichia coli*. Our findings indicate that there is a necessity to optimize the evaluation methods, especially in the direction of choosing suitable test strains and approach consistent with the further application of nanomaterials. This would ensure reliability of the results covering possible variations between the genera and strains.

This research was supported by the National Science Centre within the Project No. 2016/21/N/ST8/00095 (PRELUDIUM 11).

EFFECTS OF SEAWATER AS MIXING WATER ON PROPERTIES OF CEMENTITIOUS COMPOSITES INCORPORATED WITH NANOMATERIALS

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The dramatically increasing water consumption in concrete industry, as well as the shortage in freshwater in many parts of the world, is a severe environmental issue. Therefore, the search for alternative sources of concrete components including new water sources, e.g., recycled (from concrete production) or seawater, has gathered the attention of researchers and authorities in recent years. Particular interest was put to utilizing seawater in order to develop a durable and strong concrete. The goal of this study is to evaluate the application potential of seawater in terms of production of cement-based materials modified with nanomaterials (silica (SiO₂) and iron oxide (Fe₃O₄) nanoparticles).

Nanoparticles were suspended in seawater and analyzed with transmission electron microscopy (TEM), energy dispersive spectrum (EDS) and X-ray diffraction (XRD). Additionally, the interaction of nanomaterials with sea water was evaluated by isothermal calorimetry, as well as compressive strength development tests (1, 2, 7, 14, and 28 days).

The study showed that silica nanoparticles dissolved while mixed with seawater due to the formation of unstable silicic acid in the presence of NaCl. This phenomenon caused the uncontrolled formation of partially dissolved and agglomerated structures. Furthermore, when nanomaterials were mixed, the dissolved silica precipitated, connecting iron oxide to silica nanoparticles. Such agglomeration of nanoparticles influenced the performance of cement-based composites by hindering its hydration kinetics, thus decreasing its compressive strength development at early ages.

It was shown that the incorporation of seawater as potential mixing water for the production of cement-based composites modified with nanomaterials exhibited certain issues related to the dissolution of silica nanomaterials and the subsequent creation of agglomerates.

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MODIFICATION OF CEMENT SYSTEMS BY CARBON NANOTUBES

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The nanoparticles and nanostructures such as nano silica, nano metakaolin, titanium dioxide and aluminium oxide nanoparticles, graphite nanomaterials, carbon nanotubes of different types are used for modification of composite materials in construction industry [1, 2]. These nanoadditives allow managing by the properties of materials in fresh and hardened state. The considerable attention of researchers is focused on the investigation of cement systems modified by carbon nanotubes (CNT). The nanomodification of cement composites by CNT is determined by effectiveness of CNT homogenization in volume of dispersion and their distribution in cement matrix [3].

The present research describes the generalized data about modification of cement systems by CNT dispersion in fresh and hardened state. Modification of cement pastes by CNT dispersion leads to increase of initial setting time up to 40 min and not change the final setting time. Rheological properties of cement pastes modified by CNT dispersion are changed as well.

The modification of cement pastes by CNT dispersion demonstrates the plasticizing effect for cement pastes tested in 5 min after mixing, which did not remain after 120 min. The yield stress of nanomodified cement pastes decrease by 31 % for cement paste modified by CNT dispersion in dosage of 0.25 % by weight of cement. The maximum increase of plastic viscosity by 30% was established for cement pastes with CNT dispersion in the dosage of 0.25 % by weight of cement after 5 min of mixing. In addition the properties of cement systems modified by CNT in hardened state are changed. The density of cement mortar with CNT dispersion in the dosage of 0.25 % by weight of cement increase up to 51 kg / m³ and the flexural and compressive strength of cement mortar by 8.5 and 10.0 %, respectively. The results of experiments demonstrate the perspectives of CNT for modification of cement composites and ability to manage by the properties of cement systems in fresh and hardened state.

References

- [1] S. Kawashima, et. al. Modification of cement-based materials with nanoparticles. *Cement & Concrete Composites*, 2013, 36, 8-15.
- [2] Z. Wu, et al. Effects of different nanomaterials on hardening and performance of ultra-high strength concrete (UHSC). *Cement & Concrete Composites*, 2016, 70, 24-34.
- [3] F. T. Isfahani, et. al. Dispersion of multi-walled carbon nanotubes and its effects on the properties of cement composites. *Cement & Concrete Composites*, 2016, 74, 154-163.

SYNTHESIS OF CARBON NANOTUBES ON Ni / NiO @ Al₂O₃ CATALYSTS OBTAINED BY SOLUTION COMBUSTION METHOD

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The most common approach of synthesis of carbon nanotubes is the chemical vapor deposition method. Number of parameters, such as choice of initial carbon containing raw materials (gas or liquid), transport gas, catalyst, temperature and processing time, plays a major role in the synthesis of carbon nanotubes. As a rule, catalyst is a matrix which surface is covered with a layer of active component. In our work, the synthesis was carried out in a vertical CVD reactor using acetylene and nitrogen as initial gases with a volume ratio of 1:9 respectively. Temperature varied from 780 to 830 °C. Synthesis time is 10 min. Al₂O₃ spheres with a diameter of 0.5-1 mm and purity of 99.5 % were used as the catalyst. Nickel coating was applied on the spheres surface by solution combustion method. Firstly, initial spheres were impregnated with an aqueous solution of nickel nitrate and fuel, followed by drying and heat treatment. Citric acid and ascorbic acid were used as fuels. Preliminary studies showed that using these types of fuel enables to produce Ni/NiO nanoparticles at the ratio: 84.6 % Ni and 15.4 % NiO for citric acid as well 27 % Ni and 73 % NiO for ascorbic acid. After heat treatment, nickel/nickel oxide nanoparticles coating was formed on the surface of the spheres. Obtained carbon nanotubes were studied by scanning electron microscopy and Raman spectroscopy.

SYNTHESIS AND PHOTOCATALYTIC PROPERTIES OF NANOCOMPOSITE BASED ON MESOPOROUS TITANIUM(IV) OXIDE AND MONODISPERSE GOLD NANOPARTICLES

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Titanium(IV) oxide attracts the attention of researchers due to its photocatalytic activity and potential suitability for use in various fields of modern material science and technologies. Significant efforts of researchers are aimed at increasing the photocatalytic activity of TiO_2 , in particular, by using nano-sized TiO_2 particles and modification of its samples by metal nanoparticles. The aim of the study was to investigate the influence of gold nanoparticles on the photocatalytic activity of composite Au@TiO_2 in the process of photodegradation of methylene blue (MB) when irradiated with ultraviolet and visible light.

Nanocrystalline TiO_2 was obtained according to method described in [1]. The phase composition of the TiO_2 corresponds to anatase. It was found that size of TiO_2 crystallites is 8 nm. TiO_2 sample contains 17 nm mesopores. Stable monodisperse gold nanoparticles size of 6 nm were obtained by reduction of water solution of HAuCl_4 with sodium borohydride in the presence of histidine as a stabilizing agent. Size of the gold nanoparticles was determined by method of transmission electron microscopy. The electron absorption spectra of solutions of as-synthesized gold nanoparticles, 24 and 48 h after synthesis were measured and it was found that intensity of the absorption bands and maximum at 515 nm did not change with time. This confirms stability of the obtained gold nanoparticles with time. In order to obtain Au@TiO_2 composite the TiO_2 sample was impregnated with solution of gold nanoparticles, and excess water was removed using rotary evaporator. The solid residue was consistently washed with isopropanol and ethanol and dried at 100 °C. The final composite was content 1 % of gold. Photocatalytic activity of the Au@TiO_2 composite was investigated in the photodegradation of MB in water solution. It was found that after 60 min of UV-irradiation of the MB solutions in the presence of TiO_2 and Au@TiO_2 14 % and 56 % of MB were degraded, respectively. Under visible light irradiation in the presence of TiO_2 and Au@TiO_2 1 % and 12 % of MB were degraded. Thus, the gold nanoparticles due to the sensitizing effect improve the photocatalytic properties of the Au@TiO_2 composites both under UV and visible light irradiation.

Reference

- [1] N. I. Ermokhina, V. A. Nevinskiy, P. A. Manorik, V. G. Ilyin, V. N. Novichenko, M. M. Shcherbatiuk, D. O. Klymchuk, M. M. Tsyba, A. M. Puziy. J. Solid State Chem., 2013, 200, 90-98.

UNUSUAL MECHANICAL PROPERTIES OF HIGH-ENTROPY ALLOYS AFTER INTENSIVE PLASTIC DEFORMATION AT 77 K

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The effect of the temperature of severe plastic deformation by high-pressure torsion (HPT) on the mechanical properties and microstructure of some high-entropy alloys (HEA) was studied. For pure metals, the HPT deformation carried out at 77 K reduces the average grain size r to 70 nm (depending on HPT pressure), which is 1.5 – 2 times less than values r after HPT at ambient temperature (300 K). Lower value of average grain size after HPT at cryogenic temperatures is associated with lower dynamic recovery and higher twinning activity. Accordingly, the samples after HPT at 77 K have higher (~ 10 – 20 %) yield strength or microhardness, as well as a higher ductility compared to samples after HPT at 300 K. But it was found that in a some of HEA HPT at 77 K leads to the opposite effects – an increase the average grain size and a decrease the microhardness value in comparison with HPT at 300 K. Possible reasons for such anomalous unusual behavior are discussed.

PROSPECTS FOR USING NANOGRATING AND NANOSTRUCTURED SILICON SURFACES IN PHOTOVOLTAICS

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Using ultraviolet interferential laser lithography, rective-ion etching and chemical etching, on standard p-type silicon wafers (diameter – 50 mm, orientation (100), concentration 10^{16} cm^{-3}), technologies were developed for obtaining nanograted and nanostructured surfaces. Changing the technological parameters, it is possible to vary: the period of the nanograting from 2 to 0.3 μm , and the depth within 20 – 50 nm.

The technology of obtaining a nanograting surface was developed using the standard negative photoresist ma 2401 to obtain a nanostructured surface, a technology of selective chemical etching initiated by metal nanoclusters has been developed. The area of the nanostructured surface of silicon produced by this technology is unlimited, and the etching depth can be adjusted from a few to several hundred nanometers.

With the help of an electron microscope, the morphology of the surface of nanograting and nanostructured surfaces was studied. The uniformity of the resulting nanograte surface is satisfactory on an area of 3 – 4 mm^2 . Applying the above technology, solar cells were manufactured. They were measured: dark $I - V$, $P - V$, short-circuit current (ISH), no-load voltage (VOC), filling factor (FF), efficiency (η) and other characteristics. It was measured: work output, electrical, optical, and other characteristics of nanograted and nanostructured surfaces.

The obtained data will be used in the manufacture of solar cells of the third generation.

References

- [1] O. E. Semonin, J. M. Luther, M. C. Beard. Quantum dots for next-generation photovoltaics. *Materials Today*, 2012, 15, 11, 508-515.
- [2] Z. Zhong, K. Bosnick, J. Park, P. L. Mceuen, N. M. Gabor. Extremely efficient multiple electron-hole pair generation in carbon nanotube photodiodes. *Science*, 325, 5946, 1367-1371.
- [3] P. D. Cunningham, J. E. Boercker, E. E. Foos, M. P. Lumb, A. R. Smith, J. G. Tischler, J. S. Melinger. Enhanced multiple exciton generation in quasi-one-dimensional semiconductors. *Nano Lett.*, 11, 8, 3476-3481.
- [4] A. Tavkhelidze, L. Jangidze, M. Mebonia, G. Skhiladze, D. Ursutiu, C. Samoila, Z. Taliashvili, L. Nadaraia. Observation of geometry induced doping in thin Si nanograting layers. In: Abs. 6th Int. Conf. Silicon Photovoltaics, 2016, SiliconPV.

ORDERED GaN NANOWIRE ACCEPTOR FOR BULK HETEROJUNCTION ORGANIC SOLAR CELLS

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Solar energy is seen by many as one of the most prospective alternative energy sources, especially if one considers significant progress made lately in development of new classes of solar cells. Among others, bulk heterojunction (BHJ) based organic solar cells, utilizing π -conjugated polymer mixture with fullerene; have attracted significant attention despite relatively modest power conversion efficiency.

In this work, we report on application of self-assembled GaN nanowires grown on silicon substrate by plasma-assisted molecular beam epitaxy technique as an ordered inorganic acceptor in bulk heterojunction solar cells with active layer fabricated with poly(3-hexylthiophene-2,5-diyl) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM). Prepared organic mixture was spin-coated on top of inorganic acceptor layer, resulting structure was annealed in 150 °C for 15 min and metal contacts were deposited afterwards.

In order to investigate processes occurring on the interfaces between organic active layer, GaN nanowire and silicon, comparisons of photovoltaic devices with different inorganic acceptor layer were made. $J-V$ characteristics were measured in dark and under AM1.5 light conditions, short circuit current vs. incident light wavelength measurements were performed in the range from 300 to 1400 nm using a tungsten lamp combined with a monochromator as a light source.

Results indicate that addition of ordered GaN nanowire acceptor increases power conversion efficiency of a device compared with planar silicon acceptor, although planar GaN acceptor shows similar result. Comparison of external quantum efficiencies calculated from photocurrent shows, that efficiency of carrier collection by GaN nanowire is the highest between all measured samples. We assume existence of energy barrier on P3HT:PCBM/Si interface which explains low rate of charge carrier transfer between organic active layer and silicon substrate.

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PRUSSIAN BLUE FOR TREATMENT OF RADIOCAESIUM POISONING

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The Chernobyl nuclear reactor accident, which resulted in widespread contamination with radiocaesium, led to studies of the use of Prussian blue (PB) compounds as a countermeasure to reduce the caesium-137 and caesium-134 content of animal products. An important consideration in the practical use of PB compounds in agriculture is their possible toxicity. Studies showed that PB compounds had no adverse effects on animal health and production and, in addition, no toxic effects were noted in humans when PB was used experimentally or therapeutically.

The mushrooms can absorb high levels of the radioactive isotope caesium-137. Three decades ago the nuclear catastrophe at Chernobyl released a fair amount of caesium-137 that eventually drifted down on the Sumava mountains. The half life of Caesium 137 is 30 years – it takes 30 years for the radioactivity of the isotope to fall to half its original value. Then another 30 to fall to half again, and so on. That could cause some problems with the supply of boar meat, which is popular in the Czech Republic. A cold and snowy winter is forcing them to feed on false truffles, an underground mushroom common in the Sumava mountain region shared by Czechs, Austrians, Germans. 614 animals were inspected from 2014 to 2016, and 47 percent were above the limit [1].

PB's ability to incorporate monocations makes it useful as a sequestering agent for certain heavy metal poisons. Pharmaceutical-grade PB in particular is used for people who have ingested thallium or radioactive caesium. According to the International Atomic Energy Agency, an adult male can eat at least 10 g of PB per day without serious harm. The US Food and Drug Administration has determined the "500-mg Prussian blue capsules, when manufactured under the conditions of an approved New Drug Application, can be found safe and effective therapy" in certain poisoning cases [2]. Radiogardase (PB in soluble capsules) is a commercial product for the removal of caesium-137 from the intestine, so indirectly from the bloodstream by intervening in the enterohepatic circulation of caesium-137, reducing the internal residency time (and exposure) by about two-thirds. PB is included in WHO Model List of Essential Medicines [3].

References

- [1] U. Buntgen, M. Jaggi, U. Stobbe, W. Tegel, L. Sproll, J. Eikenberg, S. Egli. All-clear for gourmets: truffles not radioactive. *Biogeosci.*, 2016, 13, 1145-1147.
- [2] D. F. Thompson, C. O. Church. Prussian blue for treatment of radiocesium poisoning. *J. Human Pharmacol. & Drug Therapy*, 2011, 21, 11, 1364-1367.
- [3] WHO. World Health Organization Model List of Essential Medicines, April 2013, 18th List.

TWO DEFECTS MODEL OF METALS FRAGMENTATION DURING SEVERE PLASTIC DEFORMATION

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The metals are subjected to the different forms of processing for the achievement of the high mechanical properties (the high strength and plasticity). The most cardinally this purpose is reached by grinding the grain structure of the metals due to their processing by the methods of severe (mega) plastic deformation (SPD) [1]. The microdisperse structure of the grains is formed with the linear size about 100 nm as a result of such processing. Since such processing is very complex and the real experiments are rather expensive the development of the theoretical methods for their description acquires a large significance.

The general theory of the SPD process was offered [2, 3]. It is based on the nonequilibrium evolution thermodynamics which allows to describe the process of fragmentation of the polycrystalline structure of metals or alloys during SPD. As the main structural defects, the grain boundaries and the dislocations that are responsible for the formation of the fine-grained structure and the limit of the plastic flow are considered. The relation for the thermodynamic potential of the system and stationary dependencies that allow observing the formation of various limiting (stationary) structures been constructed. The study of the stability loss of stationary states of the thermodynamic system was carried out. This made possible the construction of phase diagram of metals or alloys fragmentation modes at SPD. The obtained diagram establishes the conditions for the formation of limiting structures of different types. According to obtained results a detailed investigation of the evolution of defects density and their interaction in the process of formation of various limiting (stationary) structures was conducted. The study of the phase kinetics of the defects density in the process of the formation of stationary submicrocrystalline or nanocrystalline structures was performed. The dependences of the velocity of change in the grain boundaries density on the magnitude of elastic strain were built. Thus, the optimal values for the first and second invariants of the elastic strain tensor are established, which allow to form the metal configuration with the required defects density and stable physical and mechanical properties.

References

- [1] Y. Estrin, A. Vinogradov. *Acta Mater.*, 2013, 61, 782.
- [2] L. S. Metlov. *Phys. Rev. E.*, 2014, 90, 021602.
- [3] A. V. Khomenko, D. S. Troshchenko, L. S. Metlov. *Materials Deformation & Destruction*, 2017, 8, 2.

TECHNOLOGY OF THIN FILMS OF SOME COMPOUNDS OF RARE EARTHS ELEMENTS AND MECHANICAL PROPERTIES

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Compounds of rare-earth elements draw an attention both with practical and theoretical point of view. They are convenient objects for studying fundamental the phenomenon of physics and chemistry of a solid body. In the presented work, the technology of thin crystal films GdSb_2 , TbSb , and TmTe by the method of discrete vacuum-thermal evaporation beforehand of the synthesized volume material is developed for the first time. Preparation of films was carried out at a vacuum 10^{-4} Pa. The thickness of films was $1.0 - 1.4 \mu\text{m}$. Substrates were fused silica, polycrystalline glass, monocrystalline silicon and sapphire. All films had a polycrystalline structure with lattice parameters close to parameters of the corresponding volume crystals. According to pictures of a surface of the prepared films, removed in secondary Roentgen rays, components on a surface of films are distributed evenly and, according to Auger spectrums, the structure of all films on thickness within an experimental error $\pm 0.03\text{at. \%}$ is a constant.

The method of the complete attrition determined the relative mechanical strength (RMS) of the prepared films. Experiments showed that the film RMS sharply depends on substrate material. The films prepared on a quartz substrate have the least durability, the greatest – on a sapphire substrate.

Studying the kinetic microhardness is carried out on installation DUH-211S in the loading unloading mode in the range of loadings of $1 - 1500 \text{ mN}$ by Vickers's indenter. The delay time on a maximum of loading made 10 s and at the end of unloading – 5 s . Thickness of the studied films prepared on various substrates was lonely and was $1.2 \mu\text{m}$. The maximal depth of penetration of an indenter made $1 \mu\text{m}$. Accuracy measurement of a microhardness was $\sim 3 \%$. Researches showed that the microhardness of films with increase in depth of a dimpling increases. Especially this increase is noticeable for the films applied on a substrate from sapphire then for films on a silicon substrate, and for the films prepared on a sitall and quartz substrate increases in microhardness are close to each other. Thus, the dependence of a microhardness of a film on substrate material is observed. The received results are well coordinated with literary data for the case the “weak” film on the “solid” substrate.

INTERPOLATION FORMULA FOR MAGNETIZATION OF MAGNETIC NANOFLUID

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The internal energy of the magnetic anisotropy of some nanoparticles predominates over the thermal energy even at room temperature. It is known that the magnetic anisotropy axis of the magnetic nanofluids of nanoparticles, which in the absence of a magnetic field are oriented at random, at a sufficiently strong magnetic field, are polarized along the magnetic field and the so-called mechanical anisotropy state originates. It is shown that the magnetization curve of the subsystem of polarized particles in the case, when the anisotropy energy exceeds thermal energy, has a special shape similar to the shape of a hyperbolic tangent. In the present model of a magnetic nanofluid it consists of two components (subsystems) with a variable number of particles: a subsystem of particles with randomly directed axes and subsystem of particles with polarized axes. The change of the magnetic field value causes the change of the number of particles in the subsystems followed by the change the magnetization of the whole magnetic nanofluids.

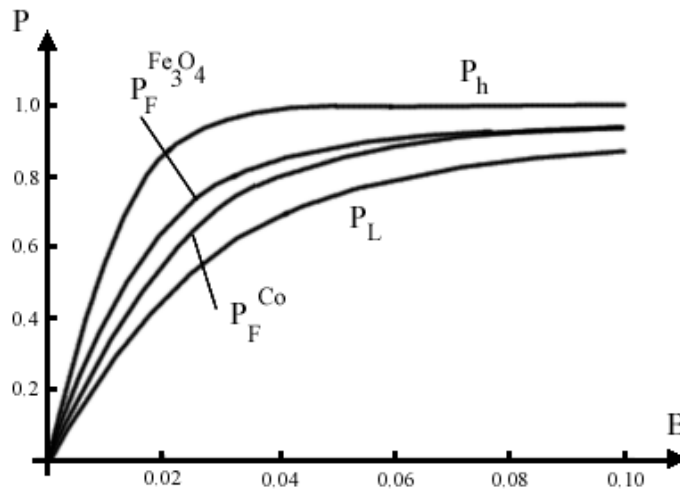


Figure 1. Magnetic polarization curves P_L , P_F , and P_h for magnetic nanofluids based on magnetite Fe_3O_4 ($d_m = 11$ nm, $a = 8.1$, $b = 78$ B) and magnetic nanofluids based on cobalt Co ($d_m = 7$ nm, $a = 20$, $b = 64$ B). In both cases there is room temperature.

For a given value of the magnetic field, interpolation formula of magnetic nanofluids magnetization is found from the condition that the chemical potentials of subsystems are equal. It is shown that the magnetization curve obtained on the basis of a two-component model of magnetic nanofluids is located between the Langevin curve and the hyperbolic tangent and with increasing anisotropy takes progressively the hyperbolic tangent shape. It is also shown that in strong magnetic anisotropy saturated state of magnetization of nanoparticles occurs much earlier than it follows from the Langevin theory. This significantly increases the Curie constant.

“GREEN SYNTHESIS” AND BIOSAFETY OF SILVER SULFIDE QUANTUM DOTS NANOPARTICLES

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Today, semiconductor quantum dots synthesis represents the strong scientific and practical interest. They have an optical spectrum that is determined by variation of dimensions, a wide luminescence excitation band, high photostability, and so on. Because of these properties, quantum dots are a promising material for photovoltaics, photocatalysis, they are used as biomarkers and sensors for medicine [1]. The reproducible method of biological synthesis of semiconductor nanoparticles of silver sulfide (I) with the mycelium of basidial fungus *Pleurotus ostreatus* was developed. It was found that absorption maxima correspond to the wavelengths at 315 and 470 nm for produced semiconductor nanoparticles. Absorption spectra are typical for Ag₂S quantum dots. In addition, morphological analysis of synthesized quantum dots was carried out using high-resolution transmission electron microscopy. The results of electron microscopy confirm the presence of semiconductor nanoparticles of silver sulfide in tested samples, they have a homogeneous, spherical morphology with a diameter in the range of 20 – 25 nm, having no surface defects. Their cytotoxic effect on bacteria of *Escherichia coli* and *Bacillus thuringiensis*, as well as on root meristems of *Allium cepa* (Allium-test), on *Drosophila melanogaster*, and human B- and T-lymphocytes were studied. Notable antibacterial activity is observed for the synthesized Ag₂S nanoparticles. When Ag₂S quantum dots were tested for antimetabolic effects (3 mg / mL), some mitotic disorders have been identified at the meta- and anaphases. It has also been established that the Ag₂S quantum dots obtained from biological synthesis do not exhibit pronounced cytotoxic effects on human B- and T-lymphocytes. At the same time, there is a slight stimulation of phagocytic activity. The result of the mutagenicity test using *D. melanogaster* demonstrates the absence of the mutagenic action of the synthesized nanoparticles. Thus, the Ag₂S quantum dots synthesized with the fungal matrix are a new promising development for biomedical research and will be used in the future as efficient and safe luminescent probes.

Reference

- [1] S. I. Sadovnikov, Y. V. Kuznetsova, A. A. Rempel. Ag₂S silver sulfide nanoparticles and colloidal solutions: Synthesis and properties. Nano-Str. & Nano-Obj., 2016, 7, 81-91.

PRELIMINARY STUDY OF NEW SHS APPROACH FOR OBTAINING NANOSTRUCTURED DISPERSE FIBROUS MANGANESE DIOXIDE

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New catalytic nano-materials are urgently needed for developing efficient rechargeable batteries with high energy density, which can withstand to the relatively high-power current pulses and a big number of charging / discharging cycles. One of the most investigated nano-materials for the rechargeable batteries is manganese dioxide. The minimum particle size of industrially synthesized manganese oxide is in the range of microns or even millimeters. Natural manganese oxide is extremely contaminated with various oxide contaminants which complicate the chemical and structural analysis of manganese dioxide and limit its applicability.

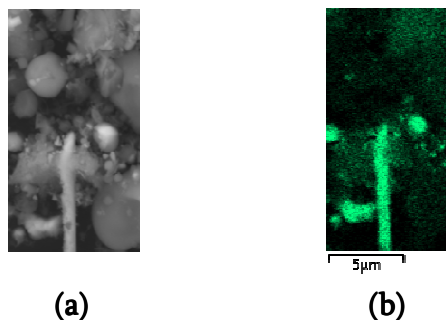


Figure 1. TEM image (a) and Mn distribution in obtained nano-structured specimen.

In the proposed work preliminary experiments on synthesis of nanostructured manganese dioxide using the method of self-propagating high-temperature synthesis (SHS) is reported.

RESISTIVE SWITCHING MODELING FOR SILICON SUBOXIDE

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Reversible resistive switching is the basis of nonvolatile memory devices called ReRAM. In most cases transition metaloxides are used as an active layer of capacitor-type ReRAM-memory cell. For such kind of active layer materials resistive switching is linked with drift-diffusion flux of oxygen vacancies in sublattice of oxygen between the two electrodes. In case of transition metals conditions at the interface between electrode and active layer and switching electric field polarity play a crucial role.

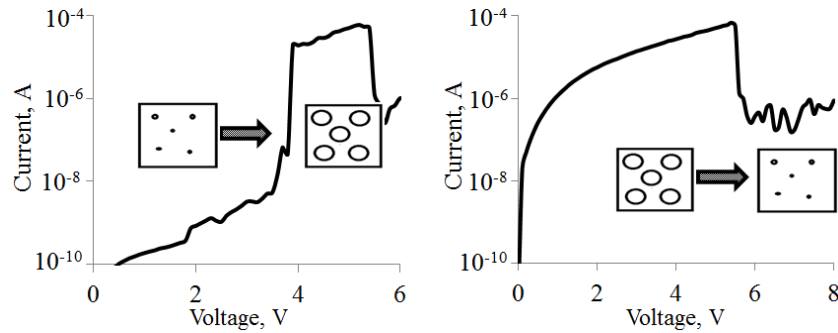


Figure 1. I – V characteristics.

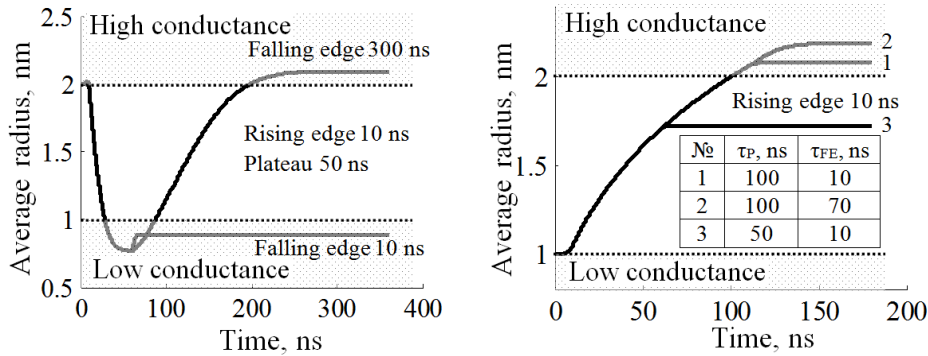


Figure 2. Average radius vs. time of switching.

This paper describes alternative solution for ReRAM based on silicon suboxide (SiO_x , $x < 2$) active layer [1] having a number of technological advantages [2]. In this case resistive switching is observed even for devices with chemically inactive electrodes such as doped silicon, poly-silicon, palladium or carbon nanotube [3] and doesn't depend on electric field polarity. The quantitative phenomenological model of the conductive filament formation and transformation in SiO_x is proposed. The model is based on quasi-chemical reactions of dot defects (SiO , VO , SiI) within bulk of SiO_x -film. These reactions lead to the formation of microfine or coarse Si-cluster ensemble in SiO_x -phase causing abrupt resistive switching (Figure 1).

The mean cluster radius dependence on the form and duration of the switching electrical pulses is obtained by means of mass balance equation solution for spherical clusters under non-isothermal conditions (**Figure 2**).

References

- [1] P. Zakharov, A. Italyantsev. Resistive switching in memory devices based on silicon oxide. *Electronic Eng. (Ser. 3: Microelectronics)*, 2015, 159, 5-10.
- [2] G. Krasnikov, et al. Silicon thermal oxidation initial stage and intermediate layer formation in Si–SiO₂ system. *Surf. X-Ray, Synchrotron & Neutron Analysis*, 2003, 2, 98-104.
- [3] J. Yao et al. Resistive Switching in Nanogap Systems on SiO₂ Substrates. *Small*, 2009, 5, 24, 2910-2915.

STUDY OF TETRA-ACID COMPLEXES WITH ANESTHETIC PREPARATION

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Anesthetic preparation trimecaine [2-Diethylamino-N-(2,4,6-trimethylphenyl)acetamide hydrochloride monohydrate (Tm·HCl)] and lidocaine [2-Diethylamino-N-(2,6-dimethylphenyl)acetamide hydrochloride monohydrate (Lid·HCl)] are one of the most generally used local anesthetics and peripheral analgesics in surgery, gynecology and dentistry. These are white crystalline powder readily soluble in water and ethanol and are used as a local anesthetic and cardiac antiarrhythmic, also for prophylaxis of sympathetic reaction during tracheal intubations. Increasing scientific evidence suggests that the purposeful synthesis and research of coordination compounds containing bio-metals and anesthesia drugs is interesting in the field of medical science and current pharmaceuticals.

We report the synthesis, structural and spectroscopic characterization of trimecaine and lidocaine complexes. Protonation of ligands takes place in the water ethanol solution of transition metal salt and Tm·HCl or Lid·HCl with any ratio, synthesized complexes of empirical formula $(\text{TmH})_2[\text{MCl}_4] \cdot n\text{H}_2\text{O}$ and $(\text{LidH})_2[\text{MCl}_4] \cdot n\text{H}_2\text{O}$, TmH⁻, LidH-cationic form of the anesthetic preparation M = Ni(II), Co(II), Cu(II); $n = 0, 1, 2$.

The composition and individuality of the complexes are determined by elementary analysis. Their solubility in water and organic solvents has been studied. To study the thermal stability and the sequence of the thermal process, the following compounds were studied: $(\text{LidH})_2[\text{CoCl}_4] \cdot \text{H}_2\text{O}$, $(\text{TmH})_2[\text{CoCl}_4] \cdot \text{H}_2\text{O}$, $(\text{LidH})_2[\text{CuCl}_4] \cdot 2\text{H}_2\text{O}$, $(\text{TmH})_2[\text{CuCl}_4] \cdot 2\text{H}_2\text{O}$. The thermograms are characterized by the DTG curve of the endo and exo-effects, which is due to their physico-chemical transformations [1]. At the first endo effect within 170 – 180 °C temperature interval, dehydration of the complexes takes place. The following endo-effects (300 – 320 °C) correspond to the oxidation of two molecules of the organic ligand of lidocaine or trimecaine. A strong exoelectric effect (560 – 620 °C) cleaves chlorine ions. In all cases, the final product of hydrolysis is metal oxide (CuO and Co₂O₃). It can be concluded that in these complexes the thermolysis process proceeds stepwise. The structure of the compounds is proposed based on infrared absorption spectrum analysis and monocrystals are characterized by X-ray diffractometer parameters [2]. In the compounds, the central ion coordination with acidoligands generates tetrahedral anion, while the ligands (Lid·HCl or Tm·HCl) in the form of protonated cations remain in an outer coordination field.

$(\text{TmH})_2[\text{CuCl}_4] \cdot 2\text{H}_2\text{O}$ crystallizes in the triclin space group P1 with $a = 12.409(2)$, $b = 13.125(3)$ and $c = 13.160(3)$ Å, and $Z = 2$, $\alpha = 119.46(2)^\circ$, $\beta = 92.15(2)^\circ$, $\gamma = 85.39(2)^\circ$, $\mu = 8.8 \text{ cm}^{-1}$, $d = 1.29 \text{ g / cm}^3$, $R = 0.046$ [3]. The structure of the island-ion type compounds is constructed from complex tetrahedral $[\text{CuCl}_4]$ -anions, (TmH)-cations and molecules of crystallization water.

References

- [1] T. Machaladze. Thermal Analysis, 2006, Tbilisi, Georg. Tech. Univ., 91 pp.
- [2] B. N. Tarasevich. IR Spectra of the Main Classes of Organic Compounds (Reference Materials), 2012,. Moscow, M. V. Lomonosov Moscow State Univ., 55 pp.
- [3] V. G. Tsitsishvili, N. B. Zhorzholiani, K .D. Amirkhanashvili. Synthesis and crystal structure of trimecaine hexachlorostannate(IV) monohydrate. Int. J. Sci. Eng. & Sci., 2018, 2, 2, 42-46.

Zn NANOPRIMING REDUCE STARCH METABOLISM IN WHEAT LEAVES

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Nanotechnology has the potential to revolutionize the agriculture and play an important role in food and crop production. Zinc nanoparticles are widely used in antibacterial, anti-corrosive, antifungal products, and their UV filtering properties can be used as one of protective adjustments in crop treatment usage.

In this study, common wheat (*Triticum aestivum* var *Podolianka*) was selected as model plant. Control group of wheat seeds were primed in distilled water (H₂O P), another two groups were primed in different concentrations of Zn nanoparticles (10 mg / L (Zn P10) and 20 mg / L (Zn P20)).

Starch metabolism in wheat plants was assessed in terms of β -amylase and α -amylase activities and total soluble sugars. The β -amylase catalyzes the hydrolysis of the second α -1,4 glycosidic bond, cleaving off two glucose units (maltose) at a time. The α -amylase is one of the key enzymes involved in degradation of starch in wheat plant and catalyzes the hydrolysis of α -1,4 linked glucose polymers to release free glucose.

After 7 days of seed germination, Zn nanopriming treatments significantly reduced α -amylase activity in wheat leaves compared with control seedlings. The α -amylase activity of leaves decreased on 31 % and 46% in ZnP 10 and Zn P20 priming treatments, respectively, compared to control (H₂O P) seedlings. The β -amylase activity in wheat leaves non-significantly changed in both Zn priming treatments.

Likewise, the total soluble monosaccharides contents of wheat leaves were reduced on 11 and 17 % by nanopriming treatments (Zn P10 and Zn P20) compared to the control.

Thus, low-concentrated zinc nanopriming significantly reduce α -amylase activity and cause non-significant changes in β -amylase activity in 7-days wheat seedlings leaves but does not cause critical decreasing of soluble monosaccharides amount in it.

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