

6TH INTERNATIONAL CONFERENCE “NANOTECHNOLOGY”

4 – 7 October 2021
Tbilisi, Georgia

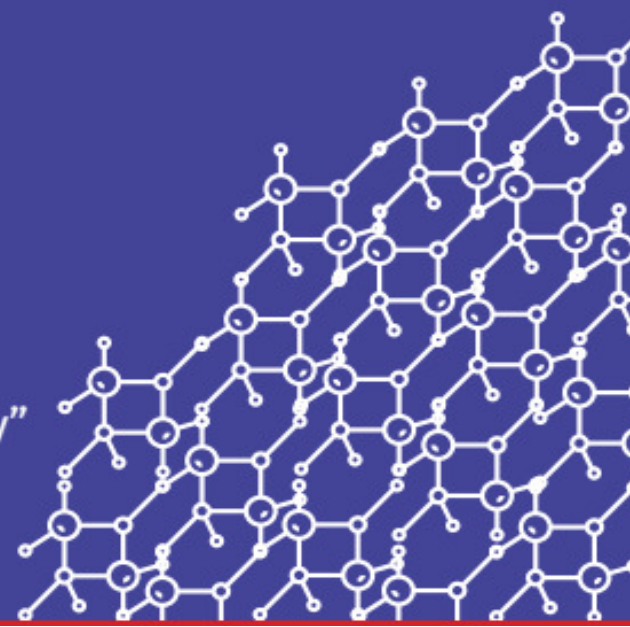
GTU nano 2021

In memory of Prof. Alex Gerasimov
initiator of GTU's nanoconferences

BOOK OF ABSTRACTS



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6th International Conference “Nanotechnology”

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G T U n a n o 2 0 2 1

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Book of Abstracts



Tbilisi
2021

Book of Abstracts contains more than 100 abstracts of papers submitted to the 6th International Conference “Nanotechnology”, 4 – 7 October 2021, Tbilisi, Georgia (GTUnano2021) organized by the Georgian Technical University (GTU). The GTUnano2021 is held in memory of Prof. Alex Gerasimov, the initiator of GTU’s regular series of nanoconferences in Georgia. The 6th conference participants represent universities, institutes, research centers, etc. leading in the field of nanotechnology and nanosciences from 20 countries (Armenia, Azerbaijan, Belarus, China, Czech Republic, Georgia, Germany, Hungary, India, Iraq, Japan, Kazakhstan, Mexico, Poland, Russia, Serbia, Spain, Turkey, Ukraine, and United States of America).

C o m p i l e r s :

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FOREWORD

Since 2010, nanotechnology conferences have been regularly, every two years, held in Georgia. Since 2012, the Georgian Technical University took responsibility for their organization and successfully held conferences in 2012, 2014, 2016, and 2018. The current – 6th Conference of this series was supposed to be in 2020, but due to the Covid-pandemic was postponed to 2021. In addition, the conference format has to be changed – now it is being held as a virtual meeting.

According to the established tradition, the 6th International Conference “Nanotechnology” will present and analyze the latest achievements not only in nanotechnology itself, but also in general, almost all the nanosciences such as: nanophysics, nanochemistry, nanobiology nanomaterials science, nanoelectronics, nanomedicine, nanoecology, nanosafety, nanoeducation, etc. We hope that at this GTU’s conference the main directions of future nano-research will be determined and the discussion held here will give a significant impact to mutually beneficial cooperation between universities and research centers of different countries in the development of new nanotechnologies. Professors and researchers in the field of nanotechnology of the GTU are ready to actively participate in the fruitful work of the conference.

The 6th International Conference “Nanotechnology” is dedicated to the blessed memory of Alex Gerasimov (1936 – 2019), the professor of our university. Professor Alex Gerasimov as scientist, teacher, and organizer of production significantly contributed of in development of nanotechnology and nanophysics, training of young personnel, and construction of the electronic industry in Georgia. He initiated the transfer of nanoconferences to GTU and then made too many efforts on their successful implementation.

In total, the conference National Organizing Committee has received approximately 105 abstracts of presentations. Among the authors are both well-known in the field researchers and promising young specialists and students. They are representatives of a number of leading universities, institutes and research centers in 20 countries (Armenia, Azerbaijan, Belarus, China, Czech Republic, Georgia, Germany, Hungary, India, Iraq, Japan, Kazakhstan, Mexico, Poland, Russia, Serbia, Spain, Turkey, Ukraine, and United States of America). All these abstracts are published in the Book of Abstracts. As for the presentations, the virtual sessions’ program includes approximately 65 invited, oral and poster presentations.

We are honored that 40 leading scientists from 21 countries have agreed to join in the conference International Scientific Committee – many thanks to them for assistance and contribution. I would also like to thank the National Organizing Committee for their hard work carried out during the preparation of the conference.

I cordially greet the participants and guests of the 6th International Conference “Nanotechnology” and wish them successful work!

David Gurgenidze

Professor

Rector of the Georgian Technical University

*Chairman of the International Scientific Committee
6th International Conference “Nanotechnology” (GTU nano 2021)*

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NOVEL SILICON SOLAR CELL FROM Ag-DOPED Sb₂O₃ PREPARED VIA THERMAL EVAPORATION TECHNIQUE

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Silver nanoparticles doped Sb₂O₃ thin films with 0.006 wt. % content of Ag and various thickness (18, 25, 28, 32, and 36 nm) has been prepared by thermal evaporation method onto glass substrates.

The Structural of the prepared films were examined from X-ray diffraction that refers to the polycrystalline films with a direction orientation (400). The Scanning Electron Microscope (SEM) images exhibits a smooth surface consisting of small spherical grain size nanoparticles. Surface analysis of Ag-doped Sb₂O₃ films examined from Atomic Force Microscopy (AFM) showed that the roughness of pure and Ag-doped Sb₂O₃ films was increased with increasing thickness.

The optical characterization has been studied in the range 200 – 1100 nm. The transmittance decreased with increasing thickness, while absorption increased. The energy gap (E_g) values decreased with increasing thickness. The $I - V$ characteristics of the Sb₂O₃ : Ag/Si devices were determined. The prepared solar cell showed a conversion efficiency of 6.8 %, a short circuit current density of 5.5 mA/cm² and an open circuit voltage of 1.25 V.

SYNTHESIS OF REFRACTORY POWDERS OF THE BORIDES OF TITANIUM AND CHROMIUM IN BURN MODE

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One of the most important directions of nanotechnology is the acquisition of nanosized powders. Changes in the fundamental properties of traditional materials in the nanodispersed state opens up a wide range of applications of nanopowders in the field of creating new materials and technologies. New materials creation with different properties and level of quality based on widely used raw materials, including man-made, is currently determined by the tasks of scientific and technological progress.

One of the main sources of boron ores in Kazakhstan are borates from the Inder deposit. These wide available raw materials can be used to obtain boron-containing refractory powder materials [1]. Popular methods of producing such materials are characterized by high energy consumption and high labor intensity. The use of self-propagating high-temperature synthesis (SHS) is currently one of the most effective approaches for creating new materials. An important role in obtaining materials in SHS mode is played by preliminary mechanochemical activation (MA), which allows achieving a high degree of particle dispersion and changing the structure, energy intensity, and high reactivity of the material [2].

To obtain samples of boride powders of refractory transition metals, mixtures containing powdered titanium dioxide, chromium oxide, enriched borate ore (boron oxide content up to 40 %) and magnesium powder were prepared. Preliminary mechanical activation of the samples was performed in the "Pulverizette-5" of a high-energy planetary centrifuge mill. The $\text{TiO}_2\text{--B}_2\text{O}_3(\text{ore})\text{--Mg}$ and $\text{Cr}_2\text{O}_3\text{--B}_2\text{O}_3(\text{ore})\text{--Mg}$ systems were selected for synthesis to produce refractory titanium and chromium boride powders. The experiments were conducted in a high-pressure reactor. After SH-synthesis the resulting powders were leached with hydrochloric acid and washed with distilled water. The products SHS were characterized using X-ray diffraction analysis and scanning electron microscopy. SHS of diborides of titanium and chromium occurred in the following reactions in the combustion wave:



The possibility of using borate ore for production nanosized refractory of titanium and chromium borides powders by method of SHS is shown.

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MICROSTRUCTURAL CHARACTERIZATION OF STRUCTURAL PHASE TRANSFORMATIONS IN SHAPE MEMORY ALLOYS

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Shape memory effect is a peculiar property exhibited a certain alloy systems with special chemical compositions in the β -phase fields, and successive displacive structural transformations govern this phenomenon. These transformations are thermal and stress induced martensitic transformations, and occurs by thermally and mechanically on cooling and stressing. Thermal induced transformations occur along with lattice twinning, and ordered parent phase structures turn into twinned martensitic structures on cooling below martensite finish temperature, and ordered parent phase structures turn into twinned martensitic structure, by means of stress induced transformation by stressing material. Shape memory alloys are deformed plastically in the low temperature martensitic condition with which and plastic strain is stored and released on heating, and recover original shape.

These alloys cycle between original and deformed shapes on heating and cooling, respectively. Thermal induced martensitic transformation is lattice-distorting phase transformation and occurs with the cooperative movement of atoms on $\{110\}$ -type planes of austenite matrix by means of shear-like mechanism. The lattice invariant shears occurs, in two opposite directions, $\langle 110 \rangle$ -type directions on the $\{110\}$ -type basal plane. This kind of shear can be called as $\{110\}\langle 110 \rangle$ -type mode, and possible 24 martensite variants occur.

By this way the twinned martensite occurs on cooling, and the twinned structure turn into the detwinned martensite by means of stress induced martensitic by deforming the material in the low temperature product phase condition. The parent phase structures turn into the detwinned structure by means of stress induced martensitic transformation by deformation in the pseudoelasticity.

Copper based alloys exhibit this property in metastable beta-phase region. Lattice invariant shear is not uniform in copper based alloys and cause the formation of complex layered structures, like 6R, 9R and 18R depending on the stacking sequences on the close-packed planes of the parent phase structure.

In the present contribution, X-ray diffraction and transmission electron microscopy (TEM) studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns 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. This result reveals the order to disorder transition in diffusive manner.

EFFECT OF COBALT OXIDE NANOPARTICLES ON ELECTRO- OPTICAL PROPERTIES OF POLYSILOXANE POLYMER

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The effect of cobalt oxide nanoparticles on electro-optical properties of liquid crystalline polymer is studied. New set of switching times were found. The effect of cobalt oxide nanoparticles on the orientation order parameter is evaluated.

HIGH HARMONIC GENERATION IN PLANE GRAPHENE QUANTUM DOTS WITH DIFFERENT SHAPES AND EDGES

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In the last decade, there has been a growing interest to extend high harmonic generation (HHG) to crystals and two-dimensional nanostructures, such as semimetallic graphene, and semiconductor transition metal dichalcogenides.

Although graphene has remarkable and unique electronic and optical properties, the lack of an energy gap greatly limits its applicability. In this aspect, graphene quantum dots (GQD) have a gap that can be controlled by its lateral size, shape, and type of edge – either armchair or zigzag. Hence, it is of interest to investigate the effect of quantum confinement on HHG in GQDs [1] by systematically varying the lateral size of a model dot.

In the present work the HHG in triangular GQDs initiated by intense coherent radiation is investigated. A microscopic theory describing the extreme nonlinear optical response of GQDs is developed. The closed set of differential equations for the single-particle density matrix at the GQD-strong laser field multiphoton interaction is solved numerically.

The obtained solutions indicate the significance of the type of edge and lateral size on the HHG process in triangular GQDs. It is shown growth in HHG efficiency with increasing confinement since the latter restricts the spreading of the electronic wave packet. This is a potential pathway to increasing yield and photon energy of HHG in nanosystems.

This work was supported by the RA State Committee of Science in the frame of the research project 20TTWS-1C010.

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HIGH HARMONIC GENERATION AT PARTICLE–HOLE MULTIPHOTON EXCITATION IN GAPPED BILAYER GRAPHENE

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Bilayer graphene is of great interest due to its rich electronic states compared to monolayer graphene [1], specifically from the point of view nonlinear interaction with the coherent radiation [2]. In particular, the real multiphoton excitation of the Fermi–Dirac sea, and highharmonic generation (HHG) by the strong laser fields in a bilayer graphene has already been justified [2, 3].

Apart from the other important electronic properties of graphene and graphene-like nanomaterials, bilayer graphene is a preferable nanosystems to realize a desire resonance with the coherent wave of certain frequency due to the widely tunable electronic bandgap with nontrivial topology. Hence, it is of interest to consider HHG process in the strong wave–bilayer graphene coupling regime with an electric field induced band gap. Moreover, 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.

In the present work, a microscopic nonlinear quantum theory of interaction of coherent electromagnetic (EM) radiation with gapped bilayer graphene (AB-stacked) is developed. The Liouville–von Neumann equation for the density matrix is solved numerically at the multiphoton excitation of the Fermi–Dirac sea. The developed theory of interaction of charged carriers with a strong driving EM wave field is valid near the Dirac points of the Brillouin zone.

We consider the harmonic generation process in the nonadiabatic and nonperturbative regime of interaction when the Keldysh parameter is of the order of unity. On the base of the results of numerical solutions, we examine the rates of odd and even high harmonics at the particle–hole annihilation in the field of a strong pump EM wave of arbitrary polarization.

Obtained results show that the gapped bilayer graphene can serve as an effective nonlinear medium for the generation of even and odd high harmonics in the THz and far-infrared domains of frequencies.

This work was supported by the RA MES State Committee of Science.

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ADSORPTION AND PHOTODEGRADATION OF QUINOLINE YELLOW, PONCEAU 4R AND BRILLIANT BLUE FCF ONTO ZnAl LDH – LDO / PVA NANOCOMPOSITE

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Because their ability to degrade organic dye compounds present in water sources, layered double hydroxide, layered double oxide and mixed oxide assisted photocatalytic degradations are attracting much attention [1].

There are several types of dyes including anionic, cationic and nonionic dyes are applied in various fields of industry [2]. All of the synthetic dyes (especially azo-dyes) can cause many human health and environmental problems and may be carcinogenic, mutagenic, etc.

Ponceau 4R – is a synthetic azo-dye (red color) with $C_{20}H_{11}N_2Na_3O_{10}S_3$ chemical formula that can be used in many food products and is normally synthesized from organic aromatic compounds. In some countries like the United States and Finland, Ponceau 4R is classified as a carcinogen and its use is prohibited [3, 4].

Brilliant Blue FCF – is a synthetic azo-dye (blue color) with $C_{37}H_{34}N_2Na_2O_9S_3$ chemical formula that can be used in food products, medications, dietary supplements, and cosmetics [5].

Quinoline Yellow WS – owing to the presence of sulfonate groups in molecule, the Quinoline Yellow WS dyes are water-soluble. It is a synthetic azo-dye (yellow color) with chemical formula $C_{18}H_{13}NO_{5/8/11}S_{1/2/3}Na_{1/2/3}$ and with a maximum absorption wavelength of 416 nm [6].

Since the anion-exchanging structure of ZnAl-based layered double hydroxide (and oxide) / polyvinyl alcohol nanocomposite (ZnAl LDH – LDO / PVA), the sorption and sunlight degradation of some anionic dyes has been studied in the present work. ZnAl LDH – LDO / PVA nanocomposite was synthesized by co precipitation-co formation method which is described in our previous work [7] found to be a very effective sorbent for cations and anions pollutants and could be used in eco-friendly environmental applications.

The bandgap energy of synthesized and applied nanocomposite is 3.2 eV which is less than the bandgap energy of pure bulk ZnO (3.3 eV). This allows photodegradation of synthetic organic dyes onto nanocomposites under lower energy radiation.

In the present work, the sorption-sunlight degradation behavior for efficient removal of quinoline yellow, ponceau 4R and brilliant blue FCF synthetic organic dyes from aqueous solution was investigated. It was found that the remove efficiency of quinoline yellow, ponceau 4R and brilliant blue FCF reached up to 91.25, 98.31 and 84.69 %, respectively, after when 0.01 g of ZnAl LDH – LDO / PVA was added into 10 mL of dye solutions which the concentration was 15 mg/L at the neutral pH condition and 298 K temperature.

In the aqueous solution, the dye anions adsorbed on the surface of the nanocomposite and intercalated in the LDH structure have undergone a photodegradation by the formed active forms of oxygen ($OH\cdot$, H_2O_2 , O_2^- and $\cdot OOH$) under sunlight (**Figure 1**).

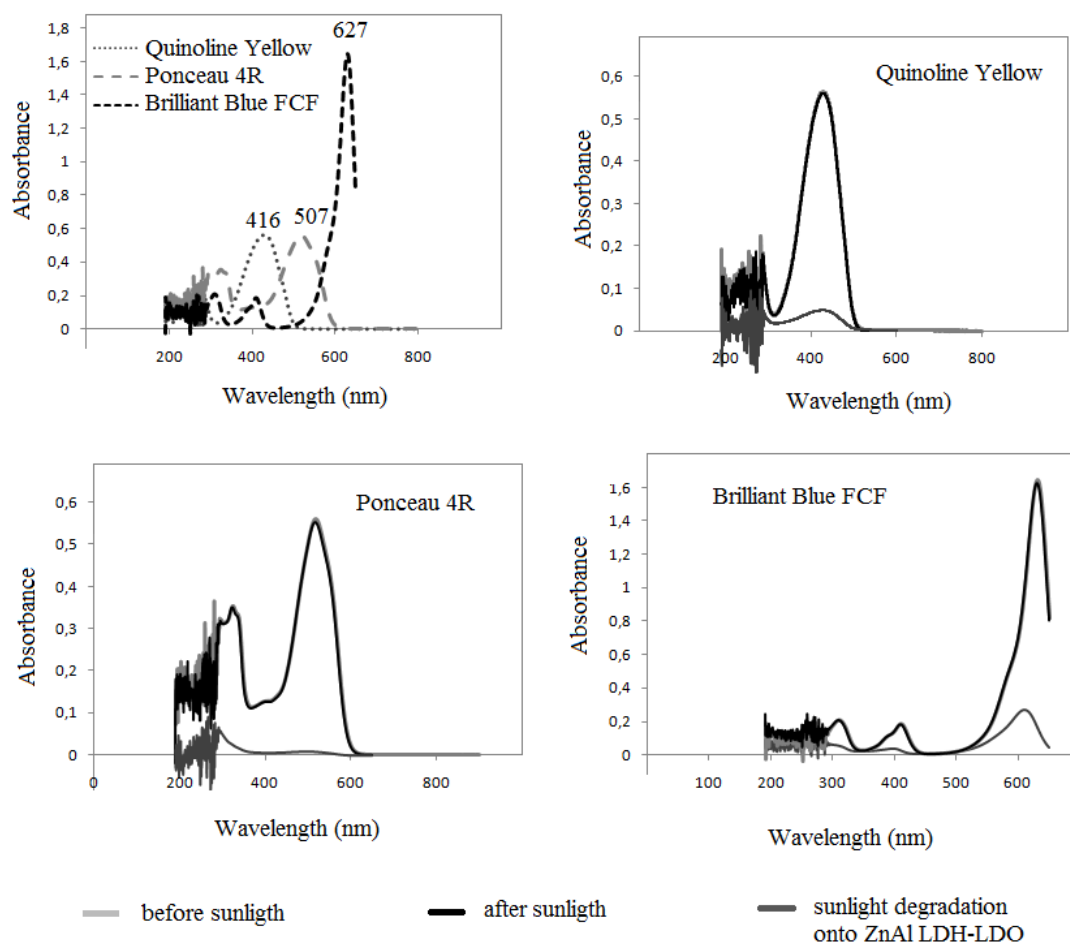


Figure 1. UV–Vis absorbance spectra of the adsorption-sunlight degradation behavior of ZnAl LDH – LDO / PVA nanocomposite for different azo-dyes.

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JOINT SYNTHESIS OF BORON CARBIDE MATRIX CERAMIC MODIFIERS AND GRAIN GROWTH INHIBITORS WITH LOW-COST COMPOUNDS

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Different compounds such as TiB_2 , ZrB_2 , W_2B_5 , WC-Co , Co are often used to increase the sinterability of boron carbide and improved physical-mechanical properties (flexural strength, fracture toughness, hardness, thermoelectric property) compared to monolithic B_4C ceramic. The method of low-temperature (1000°C) synthesis of these substances from available compounds (titanium, tungsten and zirconium oxides, tungstates, cobalt salts, organic compounds, amorphous boron) has been developed [1]. By sintering preceramic precursors using SPS method at $1300 - 1700^\circ\text{C}$, $\text{B}_4\text{C-TiB}_2\text{-W}_2\text{B}_5\text{-Co}$, $\text{B}_4\text{C-ZrB}_2\text{-W}_2\text{B}_5\text{-Co}$ and $\text{B}_4\text{C-ZrB}_2\text{-W}_2\text{B}_5$ are obtained.

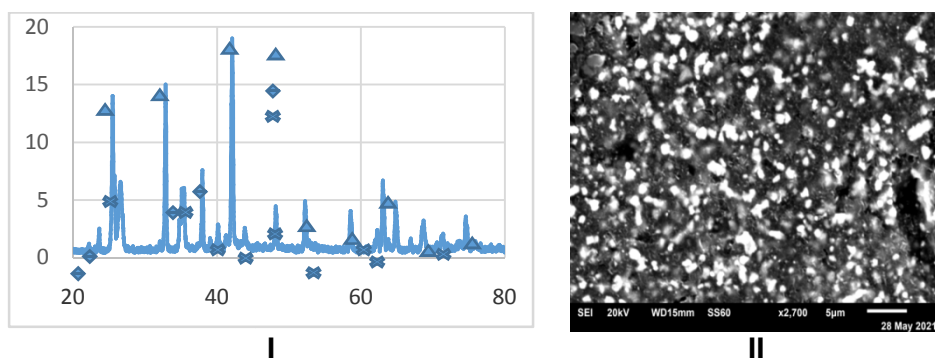


Figure 1. XRD pattern (▲ – ZrB_2 , ◆ – B_4C and x – W_2B_5) (I) and SEM micrograph of $\text{B}_4\text{C-ZrB}_2\text{-W}_2\text{B}_5\text{-Co}$ (II) composite sintered by SPS method at 1700°C .

It is established, that phases of WC-Co and W_2B_5 obtained via in situ are growth inhibitors of B_4C and ZrB_2 grains. In obtained samples using SPS method at 1700°C size of grains ranges within $0.5 - 2\ \mu\text{m}$ and they are characterized by a more uniform distribution.

This work was supported by the Shota Rustaveli National Science Foundation of Georgia (SRNSFG) – Grant # AR-18-1045: “Obtaining of boron carbide-based nanostructured heterophase ceramic materials and products with improved performance characteristics”.

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SILICON–GRAPHENE BASED SOLAR ELEMENTS

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The barrier to widespread use of sunlight to generate electricity is effectiveness and cost of photovoltaic systems. The application of materials science is essential in efforts to increase the efficiency of the light conversion and decrease the cost to levels that can compete with those for fossil or nuclear fuels. Improvements in the trade-off between cell efficiency and cost are well illustrated by the preparation of silicon wafer that is the basic material of current solar cells.

Presenting work is a continuation of the previous research of its authors dedicated to monocrystalline silicon and several kinds of thin film preparation technologies as well as creation of new semiconductor devices for different applications. It is also necessary to underline the works dedicated to shallow impurities doped monocrystalline germanium and silicon sensory systems creation (some of them with combination of graphene nanostructures is giving the unique electronic characteristics) and recently developed nanolayers based solar converter [1, 2].

Elaboration of experimental as well as modeling and simulation methodologies for preparation of silicon–graphene solar energy elements with necessary electrical and mechanical properties is the main task of the works discussing in the presented paper.

Organization of semiconductor silicon and graphene nanosystem in one sandwich for creation of new high effective photoconversion process is performed by using the silicon p-type wafer as the basis of solar converter device. The nanosize graphene nanolayer, which will be deposited on the silicon surface at its back side will play the role of charge carrier pump. Using the unique electronic and spintronic properties of graphene, its very high electric and thermal conductivity (electron mobility at room temperature – $15000 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$; measured thermal conductivity of graphene is in the range $3000 - 5000 \text{ W/mK}$ at room temperature) the silicon solar energy conversion efficiency will be fully realized in the silicon-graphene photoconversion element. All above mentioned gives the possibility for silicon–graphene device to increase the solar energy conversion efficiency up to 30 %.

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GOLD NANOPARTICLES ON InP (001) SURFACE: PREPARATION, LOCALIZED PLASMONS

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Metal–semiconductor structures with nanoparticles of metals supporting localized plasmons are of growing interest both for fundamental investigations and for applications in photovoltaics, nanophotonics, sensorics, etc. For preparation of such plasmonic structures especially promising are gold nanoparticles, possessing high chemical and physical stabilities and high quality factor of plasmon resonances.

In this work we prepare and study structures with goldnanoclusters on InP (001) surface. To prepare such structures, pieces of undopedcommercial InP wafer oriented in (001) plane were used. After rinsing in acetone, a piece of the wafer was introduced into a high-vacuum chamber, where Au film of 10 nm of thickness was thermally deposited on its surface. The formed Au/InP surface structure further underwent by annealing at 350 °C. Two 20-minute annealing stages were done. After each annealing stages, surface diagnostic was performed by Scanning Electron Microscope (SEM). The obtained SEM images show that before annealing the Au / InP surface is flat, but the annealing results in formation of gold nanoparticles on the surface. The height of the Au nanoparticles is about 12 nm, the in-surface sizes of them are in interval 20 – 30 nm.

To detect and to study localized plasmon resonance (LPR), reflection spectroscopy was used. The reflectivity spectra were measured at normal light incidence in region of the photon energy 1.5 – 5 eV. The reflectivity spectrum measured before annealing reveals only the spectral lines related with known bulk optical transitions in InP crystal. After annealing a new, intensive and broad feature appears in the reflectivity spectrum at energy of near 2 eV. The feature is assigned to localized plasmon resonance in Au nanoparticles formed on InP (001) surface as the result of annealing.

The obtained results can be used in photonic devices based on InP materials.

ELECTROCHEMICAL DEPOSITION OF NANOCRYSTALLINE Ni–Re ALLOY COATINGS

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Electrodeposition produces nanocrystalline materials when electrocrystallization results in massive nucleation and reduced grain growth. Electrodeposition is one of the most promising techniques for producing nanostructure materials owing to its low cost.

A unique complex of properties makes rhenium-nickel alloys perspective for a variety applications – electrical, catalytic, energy, etc. Ni–Re nanocrystalline deposits (5 – 35 nm) were obtained from sulfamate and citrate electrolytes for 0.3 – 5.0 A dm⁻² at 15 and 40 °C. The quantitative composition and structure of the coatings depending on the bath composition and the modes of electrolysis were determined [1]. The Ni–Re alloys contain 20 – 60 % Re if they are deposited from a simple sulfamate electrolyte, 5 – 30 % Re if they are obtained from a complex citrate bath (for 0.01 M KReO₄), and 90 – 92 % Re in the presence of 0.02 M of KReO₄. As temperature increases, the Re content of the alloy from a sulfamate electrolyte decreases.

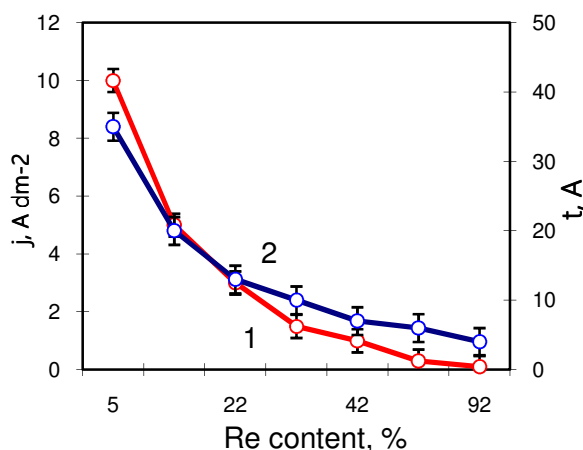


Figure 1. Correlation of the deposition current density (1) and grain size of crystallites (2) with the rhenium content in the Ni–Re deposits.

It is shown that the structure of the alloys is nanocrystalline. The grain size decreases as the fraction of Re in alloy increases (**Figure 1**).

This work was carried out in the framework of the target research program of the NAS of Ukraine “New Functional Substances and Materials of Chemical Engineering”, project №7–20, 2020.

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GEOMETRICAL SIZES EFFECT ON ELECTRICAL PARAMETERS CHARACTERIZING MEMRISTOR

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High electrophysical parameters and working sustainability of a memory storage device – memristor [1] are determined by type, thickness, and geometric sizes of its active layer. Leakage currents magnitude and as a result quality of the memristor are dependent of same factors. It is why the formation of memristor active layer with optimal parameters is considered as an important task of current nanotechnology.

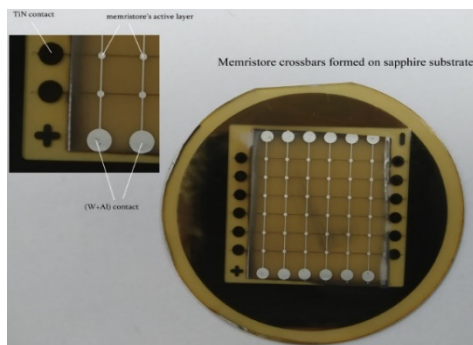


Figure 1.

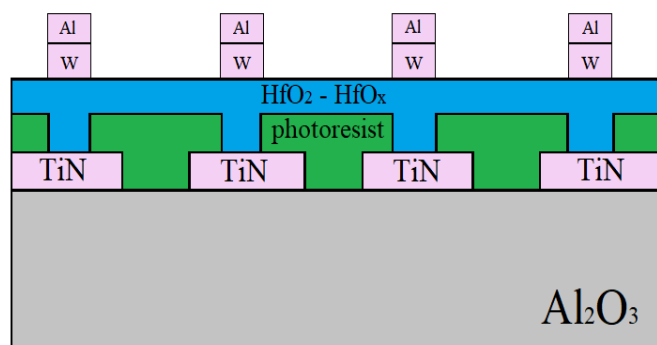


Figure 2.

There is created a memristor-structure based on hafnium dioxide [2] active layer (Figure 1). To decrease active layer in sizes it is used a photomask making it possible to reduce memristor active layer size in 400 times. 350 μm thick sapphire plates (Figure 2) are used for substrate. And contacts are made from titanium nitride / tungsten–aluminum complex. There are measured Current–Voltage characteristics [3] of obtained memristor-structure and evaluated the ratio of higher- and lower-resistances $R_{\text{off}}/R_{\text{on}}$.

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GREEN DATA COMMUNICATION: THE NEXT CHALLENGE AFTER 5G

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Since 2014 novel consumer applications like Netflix, Block Chain, ... not known to appear at the horizon have led to a huge increase of internet traffic of 60 % / year, much more than then predicted by companies like Cisco. Increased use of the internet is increasing its electrical power consumption due to increased data traffic mostly inside data centers. New centers have crossed the 500 MW level. 5G with its big jump in data speed will be another enabler for new services like LIDAR and more we cannot yet think off and will increase the energy consumption to an extent not further tolerable.

More research has to be done on the energy-efficiency of data traffic on all hierarchy levels. Inside data centers active optical cables, their electronic driver and receiver circuits and their active and passive photonic devices are coming now in the focus with the goal to minimize power consumption. Vertical-cavity surface-emitting lasers (VCSELs) for 200+ Gbit/s single fiber data transmission across OM5 multimode fiber with a record heat to bit rate ratio (HBR) of only 240 fJ/bit x wavelength @ 50Gbit/s developed in our labs are presented.

Tuning the cavity photon lifetime is demonstrated to lead to an increase of the data rate in concert with a reduction of the HBR. The VCSELs are emitting at 850, 880, 910, and 940 nm, the present IEEE 802.3 coarse wavelength multiplexing standard. Our results show, that the bit rate goals of 200, 400 Gb/s and more in the presently ongoing standardization discussions of the IEEE standardization groups can be reached alternatively by increased wavelength multiplexing leading to a reduction of the power consumption by more than 60 % as compared to reaching the data rates employing less wavelengths.

OSCILLATOR STRENGTH OF BIEXCITON EXCITED STATES IN ELLIPSOIDAL QUANTUM DOT

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Investigation of the complexes of four charged particles is of fundamental importance, especially in semiconductors, where it is possible to vary parameters in a wide range. The experimental observation of biexcitons and trions in bulk semiconductors is rather difficult because of the low binding energy [1, 2]. However, the binding energy can increase due to the effect of dimensional quantization in semiconductor nanostructures (quantum wells, quantum wires, and quantum dots) [3, 4].

In this connection, the theoretical and experimental investigation of biexciton states in quantum nanostructures is an actual problem. Semiconductor quantum dots (QDs) have a great potential for the further development of nanoelectronics due to their unique exciton–biexciton physics and the important contribution they make to quantum information processes.

The biexciton is a neutral compound quasiparticle, that is also effectively a boson and it has an integer spin when the spin-orbit coupling can be neglected. The conversion of excitons to biexciton complexes leads to various optical and other interesting effects such as change in the nonlinear susceptibility, photoluminescence emission peaks shift, etc. [5, 6]. The excited states of biexcitons also have various applications and one of them is in sharp increase in two-photon absorption. So the theoretical investigation of biexciton states in QDs is actual problem.

In this paper the excited states of biexciton states in ellipsoidal QD will be investigated theoretically. The ground state of the biexciton is a singlet state. It should be noted that the trial wave function is not symmetric with respect to electrons and holes. The variational function for the biexciton will be constructed on single-particle wave functions and will have the following form [7]:

$$\Psi_{trial}(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_\alpha, \vec{\rho}_\beta) = C \psi_{100}(\vec{\rho}_1) \psi_{100}(\vec{\rho}_2) \psi_{100}(\vec{\rho}_\alpha) \psi_{100}(\vec{\rho}_\beta) \times \\ \times e^{-\gamma \rho_{\alpha\beta}} \left\{ e^{-\lambda(\rho_{1\alpha} + \rho_{2\beta}) - \delta(\rho_{1\beta} + \rho_{2\alpha})} + e^{-\lambda(\rho_{1\beta} + \rho_{2\alpha}) - \delta(\rho_{1\alpha} + \rho_{2\beta})} \right\},$$

where C – normalization constant, $\rho_{jk} = |\vec{\rho}_j - \vec{\rho}_k|$, $j, k = \{1, 2, \alpha, \beta\}$, λ , δ and γ are variational parameters, which are determined after minimizing the integral:

$$E_{XX} = \left\langle \Psi_{trial}(\vec{r}_1, \vec{r}_2, \vec{r}_\alpha, \vec{r}_\beta) \left| \hat{H} \right| \Psi_{trial}(\vec{r}_1, \vec{r}_2, \vec{r}_\alpha, \vec{r}_\beta) \right\rangle.$$

The variational function for the excited biexciton (excited by one hole or by one electron) will have the following form:

$$\Psi_{trial}(\vec{\rho}_1, \vec{\rho}_2, \vec{\rho}_\alpha, \vec{\rho}_\beta) = C \psi_{110}(\vec{\rho}_1) \psi_{100}(\vec{\rho}_2) \psi_{100}(\vec{\rho}_\alpha) \psi_{100}(\vec{\rho}_\beta) \times \\ \times e^{-\gamma \rho_{\alpha\beta}} \left\{ e^{-\lambda(\rho_{1\alpha} + \rho_{2\beta}) - \delta(\rho_{1\beta} + \rho_{2\alpha})} + e^{-\lambda(\rho_{1\beta} + \rho_{2\alpha}) - \delta(\rho_{1\alpha} + \rho_{2\beta})} \right\}.$$

By the help of the variational method one can calculate the energy of biexciton for the ground and excited levels (**Figure 1**).

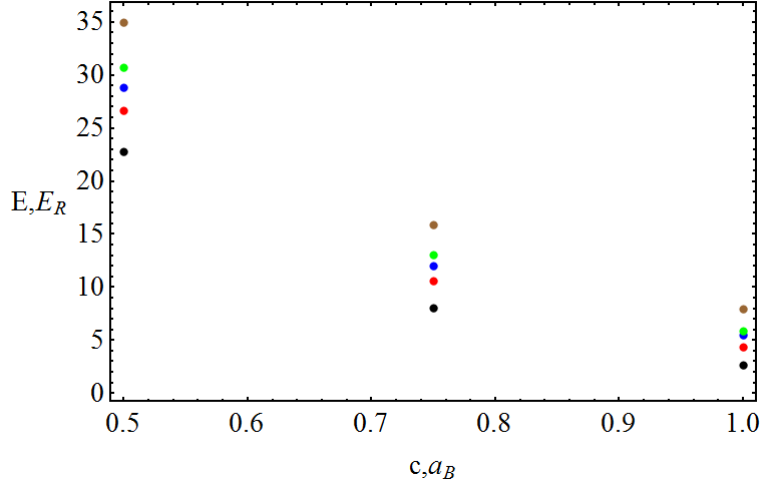


Figure 1. Dependencies of the energies of biexciton for the ground and excited levels on the small semiaxis.

Let us proceed to the calculation of the oscillator strength. The oscillator strength for the ground and excited biexcitons can be calculated using the following formula [8]:

$$f_{(xx^0, xx^1)} = A \frac{E_p}{2E_{(xx^0, xx^1)}} \left| \int_V \Psi^{0(1)}_{exc}(\vec{r}_e, \vec{r}_h) d\vec{r} \right|^2,$$

where E_p is the Keyn energy, A – recombination probability factor.

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BIOSYNTHESIS OF LUMINESCENT Ag₂S QUANTUM DOTS AND STUDY OF THEIR OPTICAL FEATURES AND GENOTOXIC EFFECTS

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Quantum dots (QDs) are semiconducting nanomaterials with unique optical and electronic properties. Ag₂S is a narrow band gap (1 eV) semiconductor with good chemical stability and optical limiting properties that has potential applications as a photoelectric and thermoelectric material [1]. The aim of this study was to synthesize Ag₂S nanoparticles by hairy root extract of *L. maroccana*, characterize their optical features and investigate their genotoxic properties on *Allium cepa* meristematic cells. “Green” synthesis was previously developed by us for cadmium-based QDs. All experimental details are presented in [2]. Photoluminescent studies revealed that for Ag₂S, synthesized by plant culture inherent spectra with maxima in the range of 450 – 520 nm depending on excitation wavelength (see Figure 1).

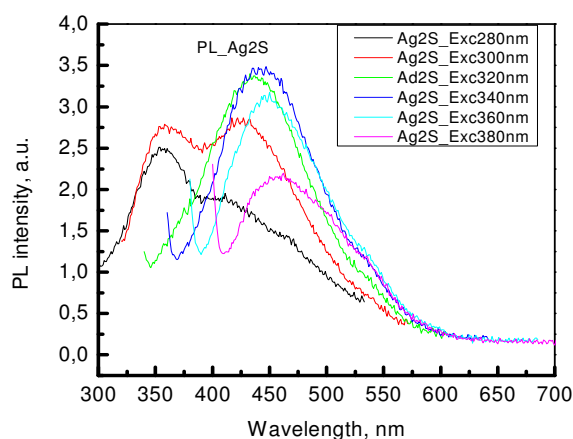


Figure 1. Photoluminescent spectra of obtained Ag₂S QDs.

It was found that Ag₂S nanoparticles did not cause significant genotoxic abnormalities in the meristem of *A. cepa* roots in concentrations from 0.3 to 3 mg/mL. The mitotic index value in the experimental samples does not differ from the control and is in the range of 91 – 99 %. It was shown that stable Ag₂S nanoparticles can be obtained by plant culture. Nanoparticles had spherical morphology, intense luminescence and were not genotoxic which allows them to be used in further cell biology studies.

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EXCITON AND POLARITON PHASES IN BUCKLED TWO-DIMENSIONAL MATERIALS

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We study the binding energies and optical properties of direct and indirect excitons in monolayers and double-layer heterostructures of Xenes: silicene, germanene, and stanene [1]. It is demonstrated that an external electric field can be used to tune the eigenenergies and optical properties of excitons by changing the effective mass of charge carriers.

Our calculations show that the existence of the excitonic insulator phase is plausible in freestanding Xenes at small electric fields [2]. We predict the formation of polaritons in Xenes, embedded in a microcavity with a movable mirror, under the action of an external electric field perpendicular to the plane of the Xene [3]. We propose that the properties of exciton–polaritons in the Xene, embedded in a variable-length optical microcavity, can be tuned by the external electric field. When an electric field is applied to a Xene monolayer, the band gap and the effective masses of electrons and holes increase, which increases the exciton binding energy [1] as well as the Rabi splitting between the upper and lower polariton branches. We analyze the dependence of the polaritonic properties, such as the Rabi splitting and cavity photon damping, on the external electric field and on the cavity length.

Furthermore, since the polariton–polariton interaction potential is determined by the binding energy and the Bohr radius of the exciton, the critical temperature of the Berezinskii–Kosterlitz–Thouless (BKT) transition to the superfluid phase is likewise tunable via the electric field. We present the conditions for a room-temperature superfluidity of lower polaritons by simultaneously maximizing the Rabi splitting and BKT transition temperature. We obtain the critical polariton concentrations for the BKT phase transition at the room temperature. Reported results contribute to the rapidly growing body of research regarding optical properties of this new class of two-dimensional semiconductors.

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SYNTHESIS OF NANOSTRUCTURE HIGH ENTROPY ALLOYS IN Fe–W–Al–Ti–Ni–C–B SYSTEM

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Multi-component alloys, in particular High-entropy alloys (HEAs) are under the interest and topic of investigations during recent years. High entropy composites introduces a new approach of developing new materials with unique properties, which is difficult to be achieved by the conventional micro-alloying approach based on only one dominant element. Different HEAs with promising properties such as increased wear-resistance, high-strength, better corrosion resistance than stainless steel and etc., have been reported. Based on the investigations, some HEAs have higher degree of fracture resistance, better tensile strength and oxidation resistance than conventional alloys. Therefore, interest towards the HEAs leads to the development of composites with improved physical and mechanical properties.

The presented work describes experimental investigations for obtaining HEAs in Fe–W–Al–Ti–Ni–B–C system. Most of the manufacturing process requires use of high temperature for extended period of time. Because of significant coarsening of the ultrafine grains, nanostructure effects are decreased. The proposed research is addressed to produce large quantity of ultrafine powders as precursors and subsequent application of explosive compaction in order to produce bulk HEAs for practical Application.

For the experiments were used powders of five major metallic and two minor non-metallic B and C elements. Mechanical Alloying (MA) technology was use for the synthesis and ultrafine / nanoblend formation from Fe–W–Al–Ti–Ni–B–C compositions which was used as precursor for the fabrication of bulk high-entropy alloy by explosive compaction (EC) technology.

For MA experiments laboratory vibrating sieve was used for sorting the initial coarse powders. The MA was realized on the high energy ball mill. Ball to powder mass ratio was 10 : 1 during MA process. Rotation speed of the jars was 500 rpm. The time of mechanical alloying was 5, 10, 14 and 28 h. The MA powders were prepared for EC experiments. After using EC technology bulk HEAs were produced and prepared for investigations.

This research was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) – grant number YS-18-063.

PROSPECTS FOR GERASIMOV'S MOLECULAR- POTENTIAL APPROACH TO NANOTECHNOLOGY

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In analogy with well-known “Molecular-Kinetic Theory”, Alex Gerasimov called his approach to the nanotechnology as “Molecular-Potential Theory”. Actually, it is not a theory, but a powerful semiempirical method allowing a quite good general description of the complex of physical properties of substances, in particular, nanomaterials. Here we briefly formulate key issues of the approach.

According to the Gerasimov's molecular-potential approach, all the properties of a substance, which is a bounded system of atoms, are determined by the chemical bonds between constituent atoms, i.e. are valence electrons in bonding or anti-bonding states. In the equilibrium, all the valence electrons are in bonding states. But, under various external influences part of them transits unto the anti-bonding states. This changes the system properties. This statement means not only thermal (heating), but all the possible types of influence, i.e. irradiation with light of relevant wavelength.

In nanomaterials, ratio of numbers of surface and bulk atoms strongly exceeds that for macroscopic specimen of same material. Accordingly, because of breaking chemical bonds in nanomaterials are palpably weakened. This explains changes in materials' properties at increasing in their dispersity, e.g. lowering of melting point in nanomaterials.

As for the validity limits, for Gerasimov's molecular-potential approach they should be defined in the near future.

ON THE MODEL OF BACTERICIDAL ACTION OF UV RADIATION

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The massive COVID-19 pandemic has spurred research into physical methods of fighting viral infection. So, in particular, the technologies of ultraviolet sterilization are being developed, the mechanisms of the effect of UV radiation on microorganisms and viruses are being investigated [1, 2]. The paper considers three approaches used in models of the effect of UV sterilization.

1. Electrodynamic. The effect of radiation on a virus is considered in the aspect of the classical problem of an electromagnetic wave incident on a spherical object, the size of which is commensurate with the wavelength [2]. The solution to the problem depends on the electrodynamic characteristics of the object, the presence of inhomogeneities in it, and the presence of free charges. The result of exposure is due to dissipative processes in the object, the effects of electrical breakdown, especially in conditions of high intensity of the electric field of the incident wave.

2. Thermodynamic. The UV radiation source is described in the absolute black body approximation, then the dose of radiation that provides the required sterilization efficiency is determined by the flux density of radiation quanta falling on the surface of an object of known dimensions. The excess of the radiation dose over the threshold level of microorganism survival provides the sterilization effect.

3. Nanotechnological. The sizes of most pathogens and viruses are in the range of 10 – 300 nm, which makes it possible to consider them as nanoparticles of a certain structure and chemical composition. Moreover, the presence, in particular on the surface of coronaviruses, of a pronounced heterogeneity in the form of clavate protein outgrowths is a factor that leads to an increase in the surface energy of the virus as a nanoparticle. It should be noted that these outgrowths are the elements that ensure the interaction of the virus with the cell and characterize the danger of the virus. From this point of view, the destructive effect of radiation can be regarded as a decrease in the level of the surface energy of a nanoparticle.

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STATISTICAL AND FOURIER ANALYSIS OF THE AUTOCATALYTIC FORMATION AND DYNAMICS OF SPATIOTEMPORAL VORTEX STRUCTURES IN FLUIDS NEAR A MAGNETIZED SURFACE

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The study of processes occurring at the magnet-electrolyte interfaces in an external magnetic field is one of the most interesting directions in the field of magnetoelectrochemistry. The hydrodynamic mixing of electrolyte during electrochemical reactions and the phase separation of electrolyte in an external magnetic field [1] are classical examples of such processes.

In our previous works, the method which had allowed to determine the characteristic frequencies of fluids motion without changing of the electrolyte structure, avoiding any distortions in the nature of the reaction, was developed (see, for example [2]). In the present study, we perform comprehensive statistical and Fourier analysis, both spatial and temporal, of the autocatalytic formation and dynamics of spatiotemporal vortex structures in fluids near a magnetized ferromagnetic surface under the influence of an external magnetic field. Using the proposed methods of analysis, we obtain integral and time dependences of the frequency distributions of fluids vortex motion over the volume under investigation. The use of the statistical analysis made it possible to detect the areas with the most intense motion of reaction products and to analyze the dynamics of the selected areas during the electrochemical reaction. By means of 1D and 2D Fourier transforms, we determine the characteristic time, spatial frequencies and the characteristic sizes of the optical inhomogeneities that occur during the electrochemical reaction.

The method of analysis developed in this work can also be applied in the cases when optical inhomogeneities and quasiperiodic motion are present in the dynamical system under investigation. The proposed method can be useful in magnetoelectrochemistry, chemical physics, chemical engineering, etc.

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SPIROPYRANS WITH NEGATIVE PHOTOCHROMISM FOR NANOTECHNOLOGY

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The last few years have seen an explosion of interest in negative photochromic systems which are coloured in their ground state and reversibly photobleach upon exposure to electromagnetic radiation with a wavelength over 400 nm, for their applications in variable transmission devices, for the development of switches, logic gates, photoregulation of drug availability, to improve prospective photochromic recording media, and to design devices with new properties, in particular, clothing and camouflage coatings that change color depending on solar light intensity. The usefulness of these systems is only gradually coming with the advantages of low energy activation.

The most interesting features in a photochromic species are the high stability and photosensitivity, fatigue resistance, and also numerous attempts have been made to achieve bathochromic shift long-wavelength absorption maximum of the colored form to radiation cheap diode laser (780 nm). In this regard, an appealing perspective is the possibility to tune or improve these properties. We have been able to increase the photosensitivity to visible light of tetrahydroquinolin spiropyran [1], and by extends π -conjugation system causes bathochromic shift of the absorption band of the coloured-zwitterionic form. The marriage of two photochromic molecule on the base of tetrahydroquinolin spiropyran and azobenzene can lead to the birth of novel hybrid material $SP_{THQ}AZ$ (Figure 1). By combining two photochromes: SP and electrophilic AZ, the length of the conjugation chain of a photoinduced form in one molecule increases resulting in the long-wave shift of the relevant absorption band.

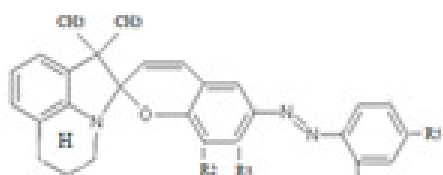


Figure 1. $R_2=R_5=$
 $=NO_2$ and $R_3=R_4=H$.

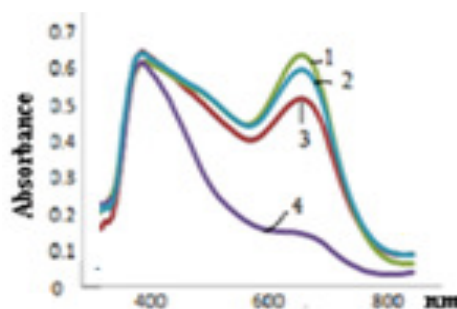


Figure 2. Absorption bands of $SP_{THQ}AZ$ in ethanol. 1 – thermodynamic equilibrium, 2 – photo chemical equilibrium, 3 – exposition light 400 nm, and 4 – after stay at daylight.

The photochromic transformation of the compound we observed at room temperature. In the compound were realized conjugation and bathochromic shift of the coloured molecule (Figure 2).

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PREPARATION OF GRAPHENE OXIDE COMPOSITES CONTAINING NANOSIZED SILVER, COPPER, AND TITANIUM OXIDE AND STUDY OF THEIR BIOCIDAL PROPERTIES

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Graphene oxide (GO, rGO) composites with nanosized metals and oxides exhibit high biocidal activity against microorganisms. Vacuum exfoliation method used [1] to synthesize rGO–Ag, rGO–Cu, rGO–TiO₂ (Anatase) composites containing 10 – 25 nm nanoparticles (Figure 1). The technique allows nanosized particles to deposit on any organic and inorganic matrix.

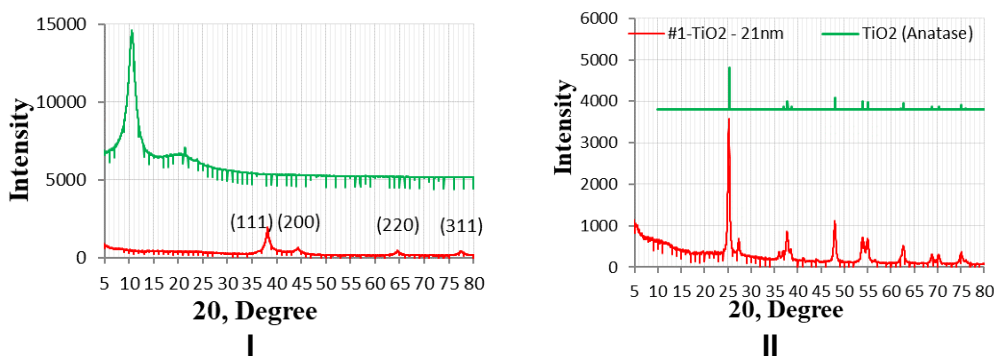


Figure 1. XRD patterns of GO (I – upper), rGO–Ag (I – lower) and rGO–TiO₂ (II – Anatase).

The antibacterial activity of graphene oxide composites (rGO–Ag, rGO–Cu, rGO–TiO₂ (Anatase)) was studied against standard test bacterial strains of Gram-negative *Escherichia coli* ATCC 25922 and Gram-positive *Staphylococcus aureus* 4399311-124.

Test cultures were incubated with 0.2 and 0.4 mg/ml of rGO–Ag, rGO–Cu, rGO–TiO₂ for 2 and 24 h to evaluate the antimicrobial effect by viable cell count and agar diffusion method. Results demonstrated that the rGO–Ag, rGO–TiO₂ fully inhibited the growth of Gram-negative *Escherichia coli* and significantly reduced Gram-positive *Staphylococcus aureus*. Nanoparticles of rGO–TiO₂ are the most effective among these metal oxide composites.

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PLAN B FOR THE CLIMATE: THE COOLING EFFECT OF ATMOSPHERIC NANOPARTICLES

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Nanoparticles could be the last remaining option to avoid overheating the earth. In the face of poverty and population growth, reducing greenhouse gas emissions is unlikely to succeed in time. Then the last remaining option is the climate control. One approach is based on radiation management with atmospheric nanoparticles. The nanoparticles lead to the formation of aerosols, which in turn trigger cloud formation. A part-per-billion concentration of appropriate substances might be enough to create clouds in otherwise cloudless regions. Clouds increase the albedo of the earth. An increase of 1 % would be enough to offset anthropogenic climate change for the time being. However, this method can have unwanted side effects. The presentation gives an overview of the current state of research.

NEW ACHIEVEMENTS IN THERMOTHERAPY

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In the field of oncology, hyperthermia (thermotherapy) is a treatment method of considerable interest also from an engineering point of view. One of the biggest problems when dealing with a malignant tumor is the spread of metastasis throughout the body in all directions. A thermal, healing deterministic effect on them can be caused by, influencing the nanoparticles inside them using electromagnetic waves.

In the course of experiments carried out by us on animals (mice) an optimal thermal treatment effect (45 – 55 °C) was achieved by nanoparticles (Fe_3O_4) using 10 kHz electromagnetic waves.

SCANNING ELECTRON MICROSCOPY STUDY OF PLASMA SYNTHESIZED NANOPARTICLES

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The commercial viability of nanomaterials strongly depends on the development of low-cost, high-performance technologies that are capable of producing nanoparticles from the inexpensive solid feedstock. The plasma arc technology that was developed by our scientific group meets this requirement and provides the means for producing different nanomaterials.

The purpose of this work was to apply the scanning electron microscopy (SEM) for the study of a morphology and size distribution of nanomaterials produced by plasma arc synthesis. Besides the SEM, the X-ray diffraction, EDX and cathodoluminescence imaging were also applied for identifying existing crystalline phases and their composition. Cd and ZnO nanoparticles were deposited by the arc plasma synthesis. The choice of Cd nanoparticles was motivated by an ongoing project devoted to the synthesis of CdS nanoparticles by direct sulfidation of metallic Cd. As for ZnO, this material in the nanocrystalline form has attracted great interest due to its wide application, which ranges from bio-medical purposes to optical and electronic usage.

It was established that the synthesized Cd nanoparticles had a spherical shape and a hexagonal close packed crystal structure with $a = 0.297$ nm and $c = 0.561$ nm. Depended on the applied plasma power their diameters ranged from tens of nanometers up to 200 nm. The spherical shapes of Cd nanoparticles indicated that before crystallization they were in a molten state and the surface tension affected their shape during solidification.

The composition and morphology of ZnO nanomaterials were greatly influenced by synthesis parameters. At a high plasma output power, the growth rate was significantly increasing causing the formation of stoichiometric ZnO nanoparticles mixed with oxygen-deficient and even pure Zn nanoparticles. At certain plasma parameters, the formation of ZnO tetrapods was observed. This type of ZnO nanomaterials is known to exhibit superior optical properties.

The results of this study showed a high potential of the developed plasma synthesis technology for producing different nanomaterials with an increased yield.

This work was financially supported by the Shota Rustaveli National Science Foundation grant AR-19-719.

PECULIARITIES OF NONLINEAR WAVES LOCALIZATION IN STRUCTURED ANHARMONIC MEDIA WITH TWO METASURFACES

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The study of propagation and the peculiarities of localization of nonlinear waves in structured (layered, modulated, periodic) anharmonic media with metasurfaces is one of the main problems of the dynamics of nonlinear waves. In the present work, we study both analytically and numerically the localized nonlinear waves propagating along two coupled parallel metasurfaces (defect layers) in anharmonic *focusing* medium in the case when metasurfaces are characterized by the refractive index that differs from that one in the matrix outside them. We consider the case when both metasurfaces are *attractive* for elementary excitations. In this case, the nonlinear wave is localized mainly at the metasurfaces.

We found the exact analytical solutions for localized *symmetric* and *antisymmetric* soliton states and demonstrate that they are governed by a *single scaling variable* that describe the ratio between the metasurface distance and the soliton state localization length. For both types of localized states, we found exactly the dependences for the *total number of elementary excitations* in the system N_λ and its *total energy* E_λ as functions of the scaling variable d characterizing the distance between the metasurfaces (**Figures 1 and 2**).

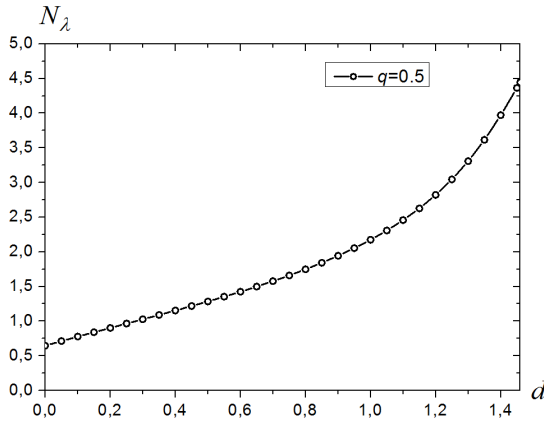


Figure 1.

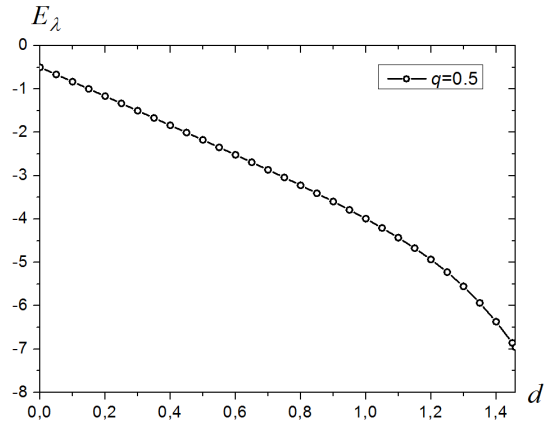


Figure 2.

We present these dependences in the *universal scaling forms* valid for different values of the metasurface “intensity” λ . We obtain numerically a monotonous behavior for N_λ and E_λ as functions of the scaling variable.

LOCALIZATION OF NONLINEAR SPIN WAVES IN A FIVE-LAYER FERROMAGNETIC STRUCTURE

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Currently, the multilayer magnetic structures are widely investigated regarding their potential technological applications. Recently, magnetic film micro- and nanostructures have been intensively studied as possible candidates for the creation of promising devices for spintronics [1] and magnonics [2]. Magnonics deals with the propagation of spin waves in magnonic crystals – artificially created periodic structures based on magnetic and, possibly, non-magnetic materials. Of particular interest are multilayer periodic (modulated) structures with ferro- and/or antiferromagnetic ordering which have pronounced anisotropic properties.

In turn, the presence of metasurfaces (thin layers) in layered structures with different magnetic properties and different ratios of layer thicknesses is the requirement for the formation of spin-wave excitations localized at the metasurfaces between the contacting magnetic layers [3, 4]. Earlier, the analysis of such excitations was limited to linear on the oscillation amplitude approximation, but now the study of nonlinear spin-wave excitations and their properties become actual. Due to the new technological possibilities of the creating of periodic nanostructures, the investigations of the propagation of nonlinear spin waves localized near thin layers of the magnetic material in a system of thin plane parallel magnetic layers (plane magnetic defects) are of great practical interest.

In the present work, we study analytically the localization of nonlinear waves propagating in a *five-layer easy-axis magnetic structure* along the alternating wide and thin layers with different single-ion anisotropies in them. We find the exact solutions for spin wave localized states, the total number of elementary excitations localized in the system and its total energy as functions of the scaling variable characterizing the distance between the plane magnetic defects. We present all these dependences in the universal scaling forms valid for different values of the characteristic of magnetic defects.

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LOCALIZED NONLINEAR WAVES AND THEIR STABILITY IN A LINEAR MEDIUM WITH COMBINED LINEAR AND NONLINEAR METASURFACE

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The investigations of dynamics and the properties of localized nonlinear waves in structured anharmonic media is always in the focus of attention of dynamics of nonlinear waves and solitons. Among others, a considerable attention is paid to theoretical and experimental investigations of spatial localization of high power electromagnetic beams in structured media with metasurfaces. The model describing an optical metasurface consisting of both linear and nonlinear parts, in a linear medium, was introduced in work [1], and the stability analysis of solitons in combined linear and nonlinear potentials according to Vakhitov and Kolokolov criterion was presented in [2].

In the present work, we study both analytically and numerically the localized states of nonlinear waves propagating along a combined linear and nonlinear metasurface (defect layer). In the framework of the nonlinear Schrödinger equation with δ -functional potential containing both linear and nonlinear spatial perturbations, we describe all possible soliton states localized near such a metasurface in optically linear medium and investigate their stability. Via the wave localization mainly at the metasurface, there nonlinear properties appear; consequently, we take into account the Kerr nonlinearity only in the defect layer.

It is demonstrated that the soliton states localized near the metasurface can exist at any sign of anharmonicity inside the defect layer in the case of attraction of elementary excitations to the metasurface. However, for the mutual repulsion between the excitations inside the layer, the localized states can exist only in the case of attraction of elementary excitations to the metasurface. For all possible localized states, the total number of elementary excitations and total energy of the system were found. We performed the analysis of stability of all localized states and found that only soliton states with attraction of elementary excitations to the metasurface will be stable.

The present study can be useful for the description of corresponding systems in optics, in nonlinear dynamics of solids, structured media with metasurfaces, in Bose–Einstein condensation, etc.

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HARMONIC GENERATION AT LOW-ENERGY PARTICLE –HOLE EXCITATION IN BILAYER GRAPHENE

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Few-layer graphene nanostructures have attracted an interest due to its unique physical properties and high degree electromagnetic (EM) nonlinearities. Bilayer graphene (AB-stacked) [1, 2] shares many of interesting properties of monolayer graphene, but provides a richer band structure. With the help of numerical simulations in microscopic nonlinear quantum theory of coherent EM radiation interaction with AB-stacked ungapped bilayer graphene, we find out the optimal values of the main parameters, in particular, for pump wave intensity, graphene temperature for practically significant case in high-order harmonics coherent emission in the particle low-energy region of the Lifshitz transitions (separation of the Fermi surface), which occurs at an energy $EL \sim 1$ meV. The Liouville–von Neumann equation is treated numerically for the second and third harmonics generation in multiphoton excitation regime near the Dirac points of the Brillouin zone. Photo-excitations of the Fermi–Dirac sea are presented when the two touching parabolas are reformed into the four separate “pockets” [1, 2]. It is shown the trigonal warping effect of peculiar properties that is crucial for even-order nonlinearity.

We examine the rates of the high-order harmonics at the particle-hole annihilation in the field of a strong pump wave of arbitrary polarization for practically real / optimal parameters of a considering system. The obtained results show that by choosing the optimal values of the main characteristic parameters, a gapped bilayer graphene can serve as an effective medium for generation of the second and third harmonics at room temperatures in the terahertz and mid-infrared domains.

This work was supported by the RA MES Science Committee.

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SENSING PROPERTIES OF SOLID SOLUTIONS $\text{Bi}_{1-x}\text{La}_x\text{Fe}_{1-x}\text{Ga}_x\text{O}_3$

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Multiferroics attract attention due to the possibility of their use in various technological applications (magnetic field sensors, magnetic memory devices, spintronics, etc.), and as object for fundamental researches. BiFeO_3 is the most known multiferroic with high values of the Neel ($T_N = 643$ K) and the ferroelectric Curie ($T_c = 1083$ K) temperatures [1]. Partial substitution of bismuth and iron allows smooth regulation of the properties of substituted ferrites.

In this work, we synthesized and investigated the sensing properties of $\text{Bi}_{1-x}\text{La}_x\text{Fe}_{1-x}\text{Ga}_x\text{O}_3$ ($x = 0, 0.05, 0.1$) solid solutions prepared by the solid-state reactions method from the corresponding oxides of high purity. Sensing properties were determined using sintered thick-film samples on ceramic substrates. Gas-sensitive element (layer) of the sensor usually had 5 – 7 mm width, 10 – 12 mm length. Its thickness didn't exceed 0.5 mm. Sensing properties were assessed by the difference in electrical resistances of sensors measured in air (R_{air}) and in air containing a certain amount of vapors of the corresponding substances (R_{gas}): $S = 100\% \cdot (R_{\text{gas}} - R_{\text{air}}) / R_{\text{air}}$.

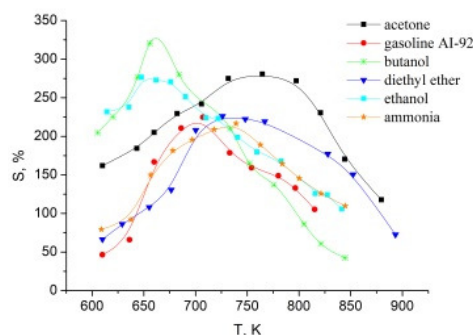


Figure 1. Temperature dependence of the response of a thick film based on $\text{Bi}_{0.9}\text{La}_{0.1}\text{Fe}_{0.9}\text{Ga}_{0.1}\text{O}_3$ in vapors of various substances.

The sensor properties of the samples were investigated for the content of ethanol, butanol, acetone, diethyl ether, AI-92 gasoline, ammonia in the air. The obtained temperature dependences of the response to the vapor content in the air had pronounced maxima in the range 650 – 750 K (**Figure 1**), which are close to the Neel temperature and correspond to the transition of the antiferromagnetic phase to the paramagnetic one. The maximum values of the response S to vapors of various substances were observed for a sample with $x = 0.1$ and varied from ~ 50 to 330 % at vapor concentrations in air up to 25000 ppm. BiFeO_3 films had the lowest sensitivity.

The results obtained indicate the possibility of using solid solutions $\text{Bi}_{1-x}\text{La}_x\text{Fe}_{1-x}\text{Ga}_x\text{O}_3$ as materials for the manufacture of gas sensors.

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PHOTOCATALYTIC PROPERTIES OF SOLID SOLUTIONS BASED ON $\text{Bi}_2\text{Fe}_4\text{O}_9$

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The discovery of the properties of a multiferroic in $\text{Bi}_2\text{Fe}_4\text{O}_9$ has led to an increase in the number of studies of materials based on this ferrite. The aim of this work was to synthesize $\text{Bi}_{1.9}\text{La}_{0.1}\text{Fe}_4\text{O}_9$ solid solution and to study its photocatalytic properties. According to X-ray phase analysis, the substitution of 10 mol % Bi^{3+} ions by La^{3+} ions in $\text{Bi}_2\text{Fe}_4\text{O}_9$ leads to the formation of the corresponding solid solution. This fact is confirmed by a slight change in the crystal lattice parameters of the orthorhombically distorted mullite structure. The photocatalytic activity of the $\text{Bi}_{1.9}\text{La}_{0.1}\text{Fe}_4\text{O}_9$ powder was studied at the room temperature by the degradation of the Acid Telon Blue dye (ATB) in an aqueous solution, under continuous stirring and exposure in the ultraviolet (UV) radiation. 100 ml of aqueous solution (in deionized water) was prepared by completely dissolving 1.0 mg of ATB dye and then dispersing 0.010, 0.020, 0.030 or 0.040 g/L of $\text{Bi}_{1.9}\text{La}_{0.1}\text{Fe}_4\text{O}_9$ powder. The ATB solution without $\text{Bi}_{1.9}\text{La}_{0.1}\text{Fe}_4\text{O}_9$ show small changes under UV-light irradiation up to 17.6 % efficiency after 90 min. The presence of 100 – 400 mg/L of $\text{Bi}_{1.9}\text{La}_{0.1}\text{Fe}_4\text{O}_9$ shows the best activity (about 37.4 %).

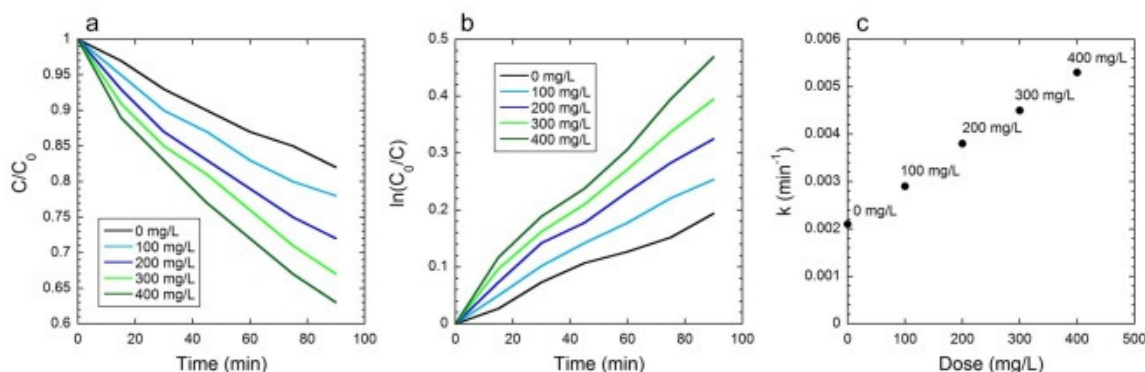


Figure 1. Residual ATB dye concentration as a function of UV radiation exposure time (a), typical plots for determining the k (b) and the k obtained for the different content of $\text{Bi}_{1.9}\text{La}_{0.1}\text{Fe}_4\text{O}_9$ (c).

We described the kinetics of the ATB decomposition reaction by the formal pseudo-first-order model as expressed in [1]: $\ln(C_0/C) = kt$, where t – irradiation time, k – reaction rate constant, C_0 – initial concentration, and C – current concentration of the ATB dye for the t . The plots (Figure 1) of $\ln(C_0/C)$ versus t exhibit approximately straight lines for the various doses showing the apparent first-order rate constants (Figure 1b). The k increases with increasing content of $\text{Bi}_{1.9}\text{La}_{0.1}\text{Fe}_4\text{O}_9$. The reaction rate constant k were 0.0053, 0.0045, 0.0038 and 0.0029 min^{-1} for the 400, 300, 200 and 100 mg/L respectively (Figure 1c). The reaction rate constant k without $\text{Bi}_{1.9}\text{La}_{0.1}\text{Fe}_4\text{O}_9$ was 0.0021 min^{-1} .

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ON THE QUANTIFICATION OF THE STRIATUM NEUROCHEMICAL PROFILE USING STEAM MRS: A COMPARISON OF 3T VERSUS 7T IN A COHORT OF ELDERLY SUBJECTS

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The primary aim of this study is to quantify the metabolite profile of the *in vivo* human striatum in a cohort of elderly subjects. Four quantification methods accounting for the effects of different experimental and / or biological parameters in the calculated concentration were compared. These included the metabolite and water MR relaxation times as well as the assumed tissue water concentration [1, 2].

More importantly, given that the partial volume effect is ubiquitous in MRS, we investigate the effect of correcting for the difference in the metabolite concentration between the different types of tissue within the MRS voxel, which is generally neglected in the literature [2]. Finally, given the lack of a gold standard technique to validate the quantified *in vivo* concentrations, the same subjects were measured at two different magnetic field strengths, 3 and 7 T, utilising different experimental protocols. The rationale behind this approach is that two or more different quantification methods leading to similar results are more likely to give results closer to the actual concentration [3].

MRS spectra were preprocessed using identical pipelines, which included removal of motion corrupted acquisitions and frequency / phase alignment of individual acquisitions [4, 5]. All spectra were subsequently quantified using the LCModel software with the basis of metabolites simulated using the density matrix formalism implemented in VeSPA [6]. Literature values for the longitudinal and transverse relaxation times, T_1 and T_2 , were used to correct concentrations for signal relaxation. Moreover, the WM / GM concentration ratio for all metabolites were assessed via linear

regression of the relaxation-corrected concentrations versus the relative GM fraction within the MRS voxel. Finally, the quantified concentrations were compared between scanners using a t-test.

In conclusion, we quantified the metabolic profile of the *in vivo* human striatum considering several potential sources of bias involved in the quantification. In particular, a full quantification of the WM / GM concentration ratio was additionally achieved.

Finally, the concentrations reached utilising two different experimental protocols at two different magnetic field strengths were compared and used as a potential validation method of the measured *in vivo* concentrations.

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LOW-SYMMETRY TWO-DIMENSIONAL STRUCTURES WITH ANISOTROPIC HIGH CARRIER MOBILITY

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A strong in-plane anisotropy of carrier transportation was found in black phosphorene [1], which provides another degree of freedom for tuning the physical properties of 2D materials and thus expands the range of opportunities for designing novel 2D semiconductors with unique applications. By combine graphene and black phosphorene, a series of previously unknown allotropes of phosphorus carbide (PC) in the stable shape of an atomically thin layer have been predicted [2].

As a result of the competition between sp^2 bonding found in graphitic C and sp^3 bonding found in black P, the PC structures can display as semi-metals with an anisotropic Dirac cone, or narrow-gap semiconductors with a strong anisotropic high carrier mobility. The relatively narrow band gaps of semiconducting PC structures can be further tuned by the approach of isoelectronic substitution. Previous unknown novel low-symmetry 2D ternary 2D structures have been designed. Sharing the geometry of 2D PC, the predicted 2D ternary structures display a strong in-plane anisotropy together with band gaps covering a wider range and broader the potential of applications in the novel nano-devices.

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SYNTHESIS AND CHARACTERIZATION OF NANO CuO-DOPED PbO THIN FILMS FOR SENSING AND SCHOTTKY DIODE APPLICATIONS

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The pure and CuO doped PbO thin films were successfully deposited on suitably cleaned glass substrate at constant room temperature, using thermal evaporation technique. The XRD results suggest that the films were crystallize in polycrystalline according to tetragonal α -PbO with a preferred orientation along (101) reflection. The AFM images confirm that all films possess a high surface homogeneity in which the distribution of crystalline granules is uniform.

The PbO film possesses a transmittance reach the 96 % inter Vis and NIR region of spectrum, and decreases with increasing the percentage of dopants reached 92 %, which is advantageous features for opto-electronic devices, especially for solar cell window layers, so it is works as filters, and antireflection coating, which reduces the energy loss in the incident radiation to its minimum value.

The optical energy gap for undoped PbO thin film is 2.87 eV while it is varies from 2.83 to 2.47 eV with increasing the percentage of CuO dopants. The best result recorded for sensitivity behavior in the case of ammonia gas is 37.5 %, which is considered as a promising result for gas sensing commercial applications. The Current–Voltage characteristics of PbO: 0.3, 0.5, and 0.7 wt. % CuO thin films exhibit the behavior of diode material.

HYDROTHERMAL SYNTHESIS AND PROPERTIES OF CHITOSAN–Ag NANOPARTICLES

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Bacterial drug resistance is a global problem of modern society. It is known that the resistance of microorganisms to metal nanoparticles and their oxides, in contrast to traditional antibiotics, is rarely occurred. In order to improve the biocompatibility and aggregative stability of nanoparticles, it seems promising to use polysaccharides (pectins, chitosans, alginates) in their synthesis, which can be used simultaneously as reducing agents and stabilizers [1]. These nanocomposites are nontoxic and biocompatible [2].

A facile hydrothermal method to synthesize chitosan-Ag nanoparticles (NPs) in aqueous solutions was developed. The chitosan with different molecular weight (from 20 to 1200 kDa) acted simultaneously as the reducing agent and stabilizer. The obtained chitosan-Ag nanocomposites were characterized by UV–Vis, FTIR and TEM. Nanocomposites had a spherical shape (**Figure 1**), their size was from 5.0 to 70.0 nm and surface zeta-potential value was over |30.0| mV. Optimal parameters (time, temperature and type of chitosan) for synthesis of chitosan-Ag NPs with the highest antibacterial activity against gram-positive, gram-negative bacteria and fungus have been determined.

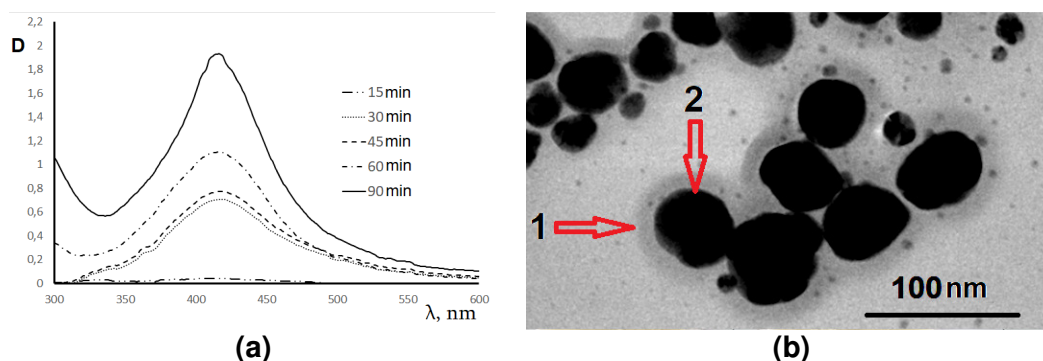


Figure 1. Absorbance spectra (a) and TEM-image (b) of chitosan–Ag NPs based on chitosan with molecular weight 30000: 1 – metal core, 2 – polymer shell.

The obtained nanocomposites are suitable for design of hybrid materials of various functional purposes, in particular, hydrogels, casting and LbL-films, 3D scaffolds.

This study was financially supported by State Committee on Science and Technology of the Republic of Belarus (project X20SERB-002).

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CHANGES IN CATALASE ACTIVITY IN PLEUSTON SPECIES UNDER THE INFLUENCE OF METAL NANOPARTICLES

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To evaluate the stress-tolerance of pleuston to the presence of metal nanoparticles colloidal solutions in water, changes in catalase activity were determined. It is widely accepted that reactive oxygen species are responsible for stress-induced damage to macromolecules and ultimately to cellular structure [1]. Catalase protect the cell from oxidative damage, transforming H_2O_2 into water and molecular O_2 [2].

Three species of free-floating on the water surface hydrophytes, so-called pleuston – *Limnobium laevigatum* (Humb. & Bonpl. Ex Willd.), *Pistia stratiotes* L., and *Salvinia natans* (L.) All. were used in our study. Cultures of aquatic plants were grown in the aquaculture complex of the NSC “Institute of Biology and Medicine” in aquariums of 40 – 60 liters in the distant water in optimum conditions: illumination of 6000 lux, the period of illumination – 12 hours, water temperature 19 – 25 °C, pH 5 – 8. Plants were exposed during 7 days on the experimental solutions of metal nanoparticles at the rate of 1 g of plant per 100 ml of the mixture of colloidal solutions of metal nanoparticles (Mn – 0.75; Cu – 0.37; Zn – 0.44; Ag^+ , Ag_2O – 0,75 mg/L) diluted 200 times. At the 7th day, a visual inspection of the plants was performed and catalase activity was determined by the method of Bach and Oparin [3].

It was revealed that catalase activity increased in two pleuston species, in *P. stratiotes* (by 19%) and in *S. natans* (by 63 %). In *L. laevigatum*, on the contrary, decreased (by 17 %). It was observed by visual inspection that species with higher catalase activity were less damaged. Among the investigated species of aquatic plants, the most resistant to the influence of a mixture of metal nanoparticles, according to the catalase activity, was *S. natans*.

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UNSTABLE PLASTIC DEFORMATION OF ULTRAFINE-GRAINED fcc AND hcp POLYCRYSTALS AT LOW TEMPERATURES

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The instability of plastic deformation, manifested at temperatures below 20 K in the form of sharp load drops and being known as low-temperature jump-like deformation (LTJD), is one of the features of the low-temperature plasticity of most metals and alloys. The information obtained in the study of mono- and coarse-grained polycrystals made it possible to formulate the basic regularities of this phenomenon [1]. However, LTJD in ultrafine-grained (UFG) and nanocrystalline polycrystals has been little studied at present. The aim of this work is to study the influence of the microstructure of the UFG polycrystals on the strain hardening rate and the scale of the LTJD.

Polycrystals of Cu ($d = 500$ nm), a solid solution of Al–Li alloy ($d = 1.5$ μm) and a magnesium alloy AZ31 ($d = 800$ nm, texture), the microstructure of which was formed by SPD (ECAH or ECAP), were studied. The samples were deformed by tension at a constant rate of 10^{-4} s $^{-1}$ at temperatures of 4.2 and 0.5 K. To study the influence of the microstructure, the initial samples were annealed at temperatures in the range 373 – 623 K.

It was found that the strain hardening coefficient θ under tension and the average stress jump $\Delta\sigma$ during LTJD substantially depend on the grain size, dislocation density and texture of the samples. As a result of SPD the grain refinement and an increase of the dislocation density lead to a decrease in θ and increase the scale of the LTJD. On the contrary, annealing is accompanied by an increase in θ and a decrease in the stress jump $\Delta\sigma$.

Thus, a change in the microstructure causes a correlated change in the parameters θ and $\Delta\sigma$, which indicates a unified dislocation-dynamic nature of strain hardening and jump-like deformation at low temperatures.

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THE SONOCHEMICAL SYNTHESIS OF PVA / Mg–Al–OH LAYERED DOUBLE HYDROXIDE NANOCOMPOSITE FILM

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Polymer nanocomposites is a class of material because of various unique properties such as improved mechanical properties, gas barrier properties, reduced flammability, increased heat distortion temperature, reduced solvent uptake, and lower flammability [1].

Last decade, layered double hydroxides (LDHs) have attracted much attention due to their easily manipulating properties and potential applications such as ion exchangers, polymer stabilizers, adsorbent catalysts [2], and their support [3], electrodes, and biomedical drug delivery [2]. Among numerous kinds of LDHs, Mg–Al–LDHs are the earliest and extensively researched products [3].

Recently, PVA-based nanocomposites have been composed to improve PVA properties and further explore its applications by the solution casting method [4].

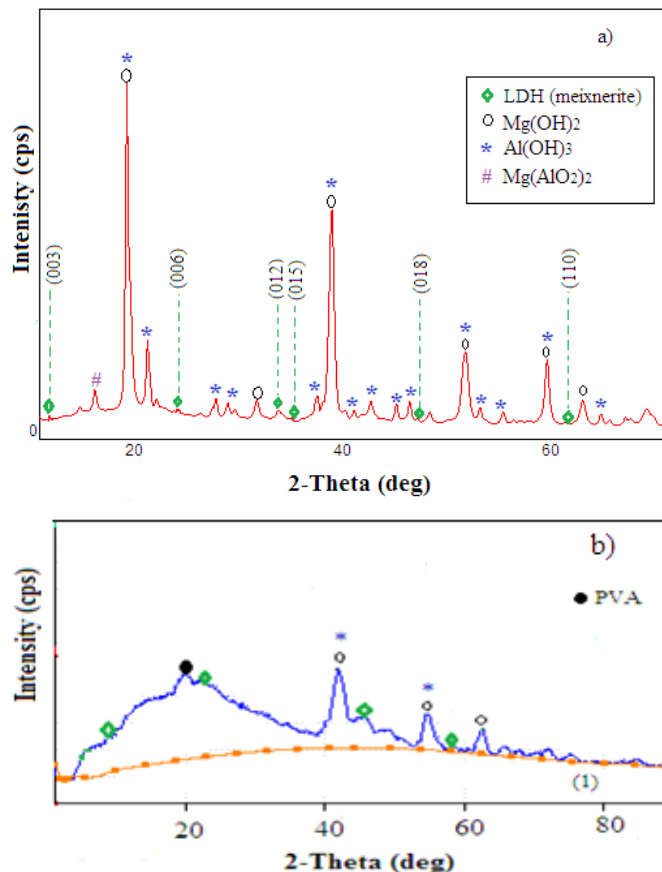


Figure1. XRD pattern of (a) Mg–Al–OH and (b) PVA / Mg–Al–OH nanocomposite film.

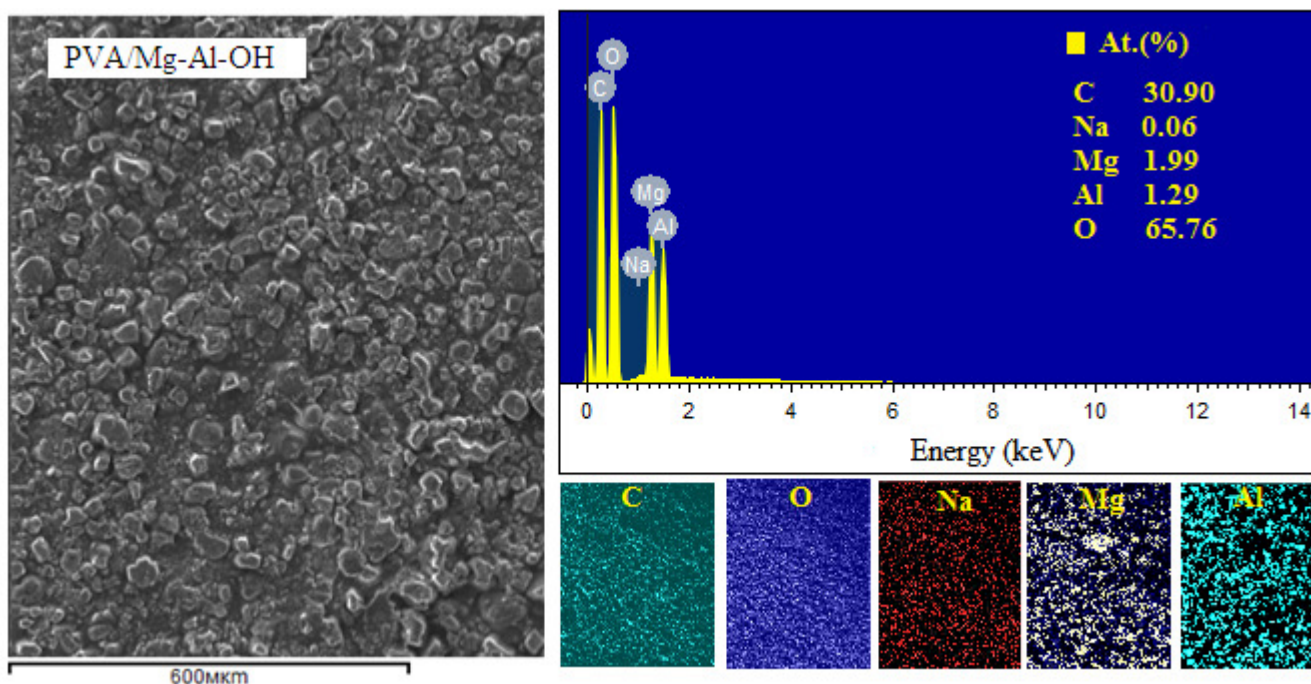


Figure 2. SEM images, EDX mapping images and EDX pattern of PVA / Mg–Al–OH nanocomposite film.

In this study, we report the synthesis of PVA / Mg–Al–OH layered double hydroxide composite film by a sonochemical method and were analyzed with physical research methods (**Figures 1 and 2**).

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SUPERCONDUCTING NANOSTRUCTURED CONCENTRATOR IN COMBINED MAGNETIC FIELD SENSOR

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In most cases, a low threshold sensitivity $\delta B \leq 1$ nT of a magnetic field sensor (MFS) is achieved through the use of superconducting film magnetic field concentrators (MFC). They reduce δB in an MFS, in which a Josephson junction, a sensor based on the spintronic effect, etc. can act as a magnetosensitive element (MSE) [1, 2]. In this work, we calculate the concentration factor of the magnetic field in a planar MFS when the active MFC bands are in both nanostructured and non-nanostructured states. **Figure 1** shows a sketch of a combined MFS (CMFS) consisting of a superconducting film as MFC and a spintronic structure as MSE.

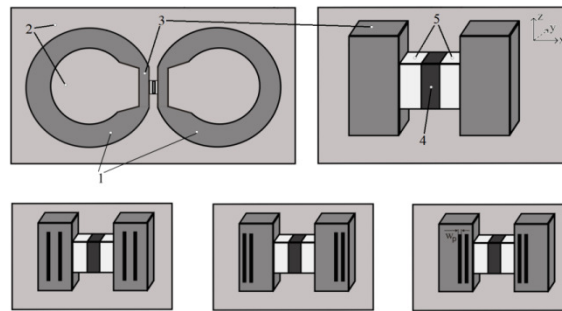


Figure 1. Schematic representation of the MFS with different positions of the slots in the active strips: 1 – superconducting ring of the MFC, 2 – dielectric substrate, 3 – active stripes, 4 – MSE and 5 – insulating film.

It was found that during the nanostructuring of the active MFC bands, i.e. the formation of parallel slits (channels) in them separating superconducting nanoscale stripes, the value of the coefficient F changes significantly. When choosing the parameters of the superconducting MFC rings (the width of the slits w_p , the distance between them, their number and mutual arrangement, the penetration depth of the magnetic field λ into the film of the active strip), the coefficient F increases by more than 2 – 3 times in comparison with the non-nanostructured (solid) active strip. The high efficiency of CMFS is realized with nanostructuring ($w_p = 20 - 50$ nm) of active bands from a low-temperature superconductor material ($\lambda \leq 500$ nm). The sensitivity of the aforementioned CMFS at an operating temperature of ~ 4 K can be of the order of 10 fT, which is comparable to the sensitivity δB for a superconducting quantum interference device (SQUID). In modern medicine, new technologies for non-invasive diagnostics and control of the operation of active implanted devices (artificial heart, various stimulants, blood flow velocity sensors, etc.) are relevant and in demand. To solve these problems, the considered CMFS can be used instead of the SQUID.

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COMPOSITE BIONANOMATERIAL FOR CREATING A STRAIN SENSOR

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In medical practice, it is necessary to control the movements of various parts of the body: limbs, joints, chest, as well as swelling, tumors, deformation of muscle tissue in the framework of postoperative therapy, etc. Strain sensors are in demand for controlling the deformation of artificial muscles or the work of artificial organs. Traditional tensoresistive sensors based on metal and semiconductor materials have a very low relative strain ($\varepsilon \leq 0.2\%$) and not a high sensitivity to deformation ($S \sim 100 - 200$). Sensors of both types are difficult to bend and, therefore, limit the movement of the biological object. We investigated prototype of the strain sensor (tensoresistor) based on the layers of the bionanomaterial contained bovine serum albumin (BSA – matrix) [1], and multi-walled carbon nanotubes (MWCNT – filler) [2].

The aqueous dispersion of 25 wt. % BSA / 0.3 wt. % MWCNT was applied by screen printing on flexible polyethylene terephthalate substrates. After drying layers by the laser irradiation (~ 970 nm) various parameters of layers were controlled, i.e. resistance R , bending angle θ , number of cycles n , measurement time, etc. One measurement cycle corresponded to a change within the range $\theta \approx \pm 150^\circ$. The layers of BSA / MWCNT bionanomaterial were mentioned: $(15 - 20) \text{ mm} \times (8 - 10) \text{ mm} \times (0.5 - 1.5) \mu\text{m}$.

The dependences of resistance R on the bending angle θ were similar for all layers: at $\theta = \pm 30^\circ$, 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 ($\sim 2 \text{ mm}$) and $d \leq 1 \mu\text{m}$, we obtained the estimate the linear strain sensitivity $S \sim 160$. The slopes of $S_\theta = (1/R_0)dR/d\theta$ of the $R(\theta)$ curves were considered to be strain-sensitivities, where R_0 is the resistance of the sensor with $\theta = 0$. It was found that with increasing the number n , R and S_θ increase and the hysteresis on $R(\theta)$ decreases. For the tensoresistor obtained: specific resistances $\sim 0.1 - 1 \Omega\cdot\text{m}$, $S_\theta \sim 1.0 - 1.5\% / \text{grad}$. These results are high.

In the previous, as well as in the present work, we were able to change the resistivity of the bionanomaterial depending on the mode (pulsed, continuous) and laser radiation power [3]. This allows you to get the parameters of the strain sensor to the desired values. The examined layers of the bionanomaterial BSA / MWCNT as a strain sensor is of a particular interest for medical practice. In particular strain sensors can be implemented by applying a water dispersion of nanomaterials to human skin using a 3-D printer for monitoring: movements (arms, blinking) and detection of signs of pathology (dysphagia, respiratory diseases, angina, et al.).

This study was supported by the Russian Science Foundation, project no. 18-79-10008.

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INFLUENCE OF THE MAGNETIC FIELD GRADIENT ON THE OPTICAL DENSITY OF AN AQUEOUS DISPERSION CONTAINING BIOLOGICAL MATERIAL AND CARBON NANOTUBES

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Composite nanomaterials containing matrices of biological materials and filler made of carbon nanotubes (CNTs) are promising. They can be used in various implants, for example, in bone or cartilage tissues, and their aqueous suspensions, the so-called biological solders, are suitable for laser welding of biological tissues [1].

Since CNTs contain catalytic ferromagnetic or so-called superparamagnetic nanoparticles, they can be used for non-invasive monitoring of nanotubes. Thus, carbon nanotubes can be regarded as a kind of magnetic particles (MPs).

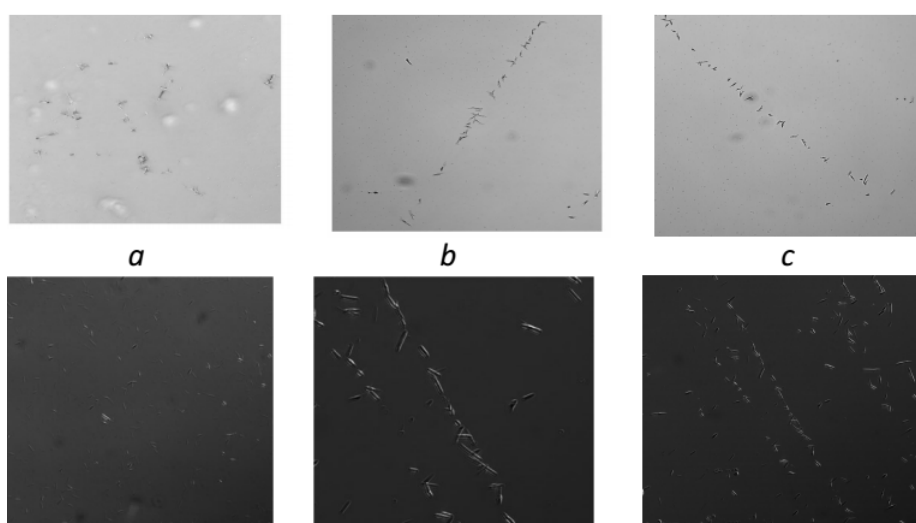


Figure 1. – Typical pictures of films on glass substrates in a confocal microscope:
a – before the action of a magnetic field (light and dark fields) on the dispersion;
b and **c** – after exposure of the dispersion in a magnetic field (light and dark fields in different parts of the film). Everywhere magnification is 200.

In our experiment (**Figure 1**), we investigated the change in optical transmission under the action of the magnetic field of aqueous dispersions containing biological materials and single-walled CNTs (SWCNTs).

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INFLUENCE OF THE SURFACE MAGNETIC BARRIER ON THE CRITICAL CURRENT IN NIOBIUM FILMS AND THE POSSIBILITY OF CREATING A HIGHLY SENSITIVE ANGULAR DISPLACEMENT SENSOR

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The free penetration of magnetic field B into the interior of the superconductor is impeded by the magnetic barrier that exists on its boundary. A typical barrier is the so-called Bin-Livingstone magnetic barrier (MB) arising due to the interaction between the Abrikosov magnetic vortex located near the boundary of a type II superconductor and its mirror image located near the outer boundary of a superconductor [1]. The type II film superconductors have a boundary MB arising either on their surface MB (SMB) in a parallel magnetic field B , or on the edges (EMB) in a perpendicular magnetic field. Both SMB and EMB can strongly influence the value of the critical current I_c and its dependence on the external magnetic field $I_c(B)$.

In this regard, the dependence of I_c on B was studied at various angles θ between the film surface and the external magnetic field. The samples were single crystal (heteroepitaxial layers, HEL) and polycrystalline (PC) Nb films on sapphire. The films were deposited by condensation from molecular beams in an oil-free vacuum of $5 \cdot 10^{-5}$ Pa on sapphire substrates with electron-beam evaporation of Nb. The films had the following dimensions and shape of the bridge: thickness – 80 – 85 nm, width – $w = 50 - 300$ μm , length – 2 mm, coast of the bridge – 3×3 mm.

It was found that for all films, regardless of the degree of their structural perfection, the value of w is one of the parameters determining the possibility of a dominant influence of MB on the type of $I_c(B)$ curves. For films, the upper limit of this possibility is the width $w \leq 200 - 250$ μm , at which the influence of SMB on $I_c(B)$ is reflected, and at $w \geq 200 - 250$ μm . These effects are as follows: $\theta = 0$ (B is parallel of the film surface), and $\theta \geq 30^\circ$, the dependences $I_c(B)$ are monotonic, which is caused by the action of EMB. In another region $\theta \sim \pm 8^\circ$ on $I_c(B)$, the curves show nonmonotonic regions with maxima and minima, which is a consequence of the influence of SMB on the critical film current. Apparently, in this case, the magnetic vortices break off from the surface and abruptly enter the film, therefore, a sharp drop in I_c and the appearance of a section with a high slope on $I_c(B)$ are observed.

It has been shown that it is possible to create a highly sensitive angular displacement sensor (resolution $\Delta\theta \leq 0.1$ angular seconds, dynamic measurement range > 100 dB in area $|\theta| < 2^\circ$) with optimal selection of HEL and PC niobium film parameters when magnetic barriers exist on its surface and edges. It should be noted that the value $\Delta\theta$ takes on a lower value in HEL than in PC films. Apparently, this is due to the fact that HELs have more perfect and smooth surfaces relative to the surfaces of PC films. The highly sensitive angular deviation sensor will be in demand in medical applications and in various fields of technology for precise orientation in space. Apparently, with the help of the proposed sensor, it is also possible to record the location of the magnetic marker in the body with high accuracy.

This work is supported by the Ministry of Science and Higher Education of the Russian Federation (project No. 075-03-2020-216 of December 27, 2019).

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PENETRATION DEPTH OF ELECTROMAGNETIC WAVE IN NANOPARTICLES

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One of the biggest challenge in nanotechnology is to understand how the nanoparticles (NPs) may be tailored by altering their size, shape and material composition, and what influence the environment has on their scattering and absorption properties, as well as on the penetration depth of electromagnetic (EM) wave in NPs, to develop novel methods for medical applications [1] and to design novel antennas, sensors, waveguides and lasers [2].

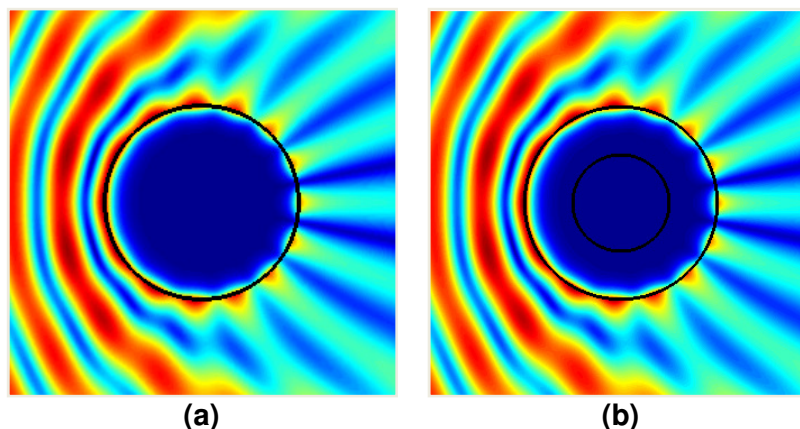


Figure 1. Near-field amplitude of magnetic field for Ag ($\epsilon = -4.42 + 0.73 i$, $R = 400$ nm) NPs illuminated by EM wave ($\lambda = 413$ nm) along (1,0) direction: **(a)** Ag NP and **(b)** SiO₂ / Ag core / shell NP.

In this work the penetration depth as function on various NP parameters is investigated in conjunction with the development of new spectral Surface Integral Equation (SIE) methods to study optical response of NPs. Promising results, obtained by us with spectral Boundary Integral Equation (BIE) methods used for solving two-dimensional (2D) problems for plasmonic application [3] and successful attempts in developing their 3D analogies with SIE based techniques lead us concluding that spectral SIE method as well as Method of Auxiliary Sources (MAS) [3] will be the most efficient and reliable methods for 3D analysis of objects in nanotechnology. It is clear already with 2D analysis of simple NPs, that EM field does not penetrate completely in Ag NP, and not even affected by the presence of SiO₂ ($\epsilon = 4.5437$) core, when Ag NP became Ag shell (**Figure 1**), leading to ideas of producing noble metal NPs in economic way, embedding cheap core inside of expensive shell. The sets of various NPs are investigated.

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SURFACE PLASMON RESONANCE WAVELENGTH OF NOBLE METAL NANOPARTICLES

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Noble metal nanoparticles (NPs) are known to have unique optical properties. Their illumination by a light source may result in strong resonant scattering and/or absorption of light along with high optical field enhancements [1]. Powerful near-field enhancements are results of resonant oscillations of the free electrons confined to the nanoparticles' surface. This resonant wave motion phenomenon is known as surface plasmon resonance (SPR).

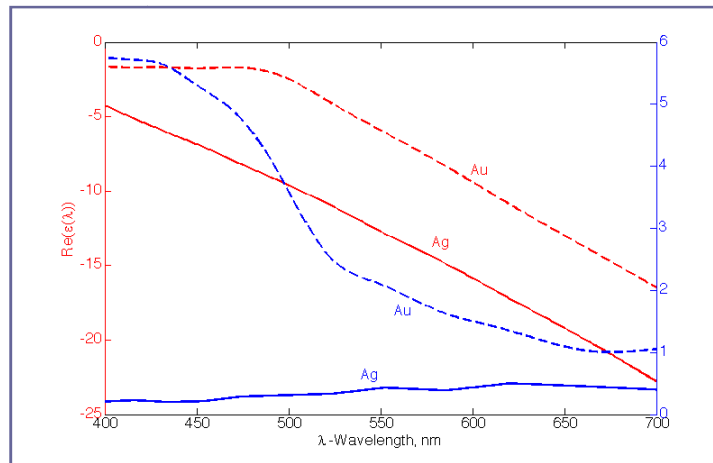


Figure 1. Functions of dielectric permittivity on wavelength for gold and silver.

The application area of SPRs is very broad and the effectiveness of NPs for each particular application depends strongly on their optical response at SPR. To find the SPR wavelength and to study optical response for each particular application in this work the new algorithm based on spectral Boundary Integral Equation (BIE) method [1] in conjunction with the methods of algorithmic differentiation [2], including Newton's method, Halley's method and method of the third order, are developed. When Newton's method was used to find resonant wavelength for hexagonal dielectric resonators [3], where dielectric permittivity is assumed to be constant, in this work one takes into account that dielectric permittivity of gold and silver are the complex valued functions on wavelength (Figure 1). The set of results demonstrates the perspective to use NPs for early diagnostics in medicine and for detection of pollutants in ecology.

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TERBIUM MONOTELLURIDE NANOFILMS TECHNOLOGY AND SOME ELECTROPHYSICAL PROPERTIES

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Monochalcogenides of rare-earth elements have interesting electrophysical, magnetic, optical, thermal, mechanical and other properties, but not all compounds of this class are studied fully. TbTe belongs to such little-studied materials.

The purpose of this work was to develop the technology of nanofilms TbTe on various substrates and the study the dependence of the electrical resistance and the concentration of charge carriers on the characteristic particle sizes of films. 0.2 – 0.8 μm thick films were prepared by vacuum-thermal evaporation from two independent sources of Tb and Te. Evaporation of terbium was carried out electronically by electron-beam evaporation and tellurium by the Joule evaporator. In the course of a dusting temperature of the evaporator of terbium equaled ~ 1600 K, and a tellurium ~ 780 K. Distances from Tb and Te evaporators to a substrate made, respectively, 22 and 43 mm. Speed of a dusting of films was equal to 55 $\text{\AA}/\text{s}$. Temperature of a substrate changed within 720 – 1150 K. As substrates we used glass-ceramic, fused silica, sapphire and (111) – oriented single-crystal silicon plates. Optimum temperature of a substrate is 1110 K, above this temperature the besieged atoms come off a substrate, and below the temperature the adsorbed atoms create islands of various thickness.

According to the X-ray analysis a film had structure of NaCl-type with lattice constant 6.10 \AA and according to the X-ray microanalysis films contained 50.1 at. % of Tb and 49.9 at. % Te. The picture of TbTe surface has been removed by electronic-scanning microscope. This process has shown that the film contains characteristic elements with the size range within 24 – 49 nanometers, that allows to draw a conclusion that we have nanodimensional object, ~ 80 % of grains have a diameter of 32 nm.

Experiments have shown that with an increase of the temperature of the substrate, the size of grains as well as the lattice constant increases. Measurements showed that the temperature of specific electrical resistance of films increases with increasing grain size and the concentration of charge carriers decreases.

UNCONVENTIONAL METALLIC PHASES IN A QUANTUM WIRE WITH MODULATED SPIN–ORBIT COUPLING

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In our early studies it was shown that a spatially modulated Rashba spin–orbit coupling in a quantum wire drives a transition from a metallic to an insulating state when the wave number of the modulation becomes commensurate with the Fermi wavelength of the electrons in the wire [1, 2].

In the given presentation we discuss extended versions of these studies, where the commensurability effects are violated by additional perturbation what opens a window for realization of unconventional metallic phases. In particular, we show that the combination of a uniform magnetic field and a gate voltage controlled spatially modulated Rashba spin–orbit interaction may drive a quantum wire into a *half-metal* phases. In the half-metal phase, electrons with only a selected spin polarization exhibit ballistic conductance, while electrons with opposite spin projection are blocked in an insulating phase. We also show that the commensurability conditions for the appearance of half-metal phase can be tuned by varying the magnetic field. These results hold promise for the design of a magnetic field-controlled spin-filter device, without resorting to injection from ferromagnetic leads [3].

We also show that the combined action of a Dresselhaus spin-orbit coupling, that is generically present in a quantum wire embedded in semiconductor heterostructure, and of a spatially periodic Rashba interaction leads to the formation of a *helical metallic phase* in a quantum wire in the limit of strong electron–electron interaction. In the helical-metallic phase of a quantum wire, electrons with opposite spin polarization move in opposite directions. The effect is sustained by a helicity-dependent effective band gap which depends on the size of the Dresselhaus and Rashba spin–orbit couplings [4].

The design for corresponding semiconductor device in which the half-metal or the helical-metal phase can be realized is briefly discussed.

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PHOTOSTIMULATED DIFFUSION OF Mn IN Si

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Mn-doped Si has a number of unique properties that make it possible to develop and create fundamentally new classes of devices for functional electronics and sensors of physical quantities. Standard high-temperature diffusion of Mn into Si: does not allow one to obtain samples with a stable state of Mn atoms in the lattice; leads to significant erosion of the surface and the formation of various silicides of the SiMn type in the near-surface region of the material; complicates the use of some interesting phenomena observed in Mn-doped Si in electronics.

We have made studies in which the diffusion of Mn into Si was carried out by means of pulsed-photon irradiation (PPI) instead of the traditional high-temperature diffusion processes. PPI was performed on the original system which allows efficient conduction of the said process. PPI system consists of two units: a control unit and a radiation unit. The use of the Π -shaped reflector design, and the radiation source of a set of 19 KG 1000 x 220 hallogenic lamps arranged in two rows, ensures uniform irradiation of the samples throughout the area of 100 cm². The system allows a smooth change in the irradiation power density up to 190 W·cm⁻², and the pulse duration from 0.1 to 1000 s in 0.1 s increments. The temperature of the samples, depending on the physical or technological task, is controlled by selecting holders and venting heated air. In order to avoid uneven heating of the sample over the entire the area to reduce the local places of heat removal, the contact of the crystal with the holder should be minimal or continuous over the surface. This is achieved by placing the samples in the reflector block on quartz needles or on a copper holder with a polished surface. The design of the copper holder provides its cooling with running water or liquid nitrogen vapour.

The starting material was p-type single-crystal Si (B) plates ($D = 50$ mm) with a resistivity of $\rho = 1$ Ohm·cm. The sources of diffusion were: 50 % aqueous solution of manganese chloride ($\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$); 50 % aqueous solution containing pure manganese; $\text{Mn}(\text{NO}_3)_2$ solution. Ohmic contacts were obtained by depositing 0.5 μm thick Al film with subsequent PPI. The following parameters were measured: conductivity type; surface resistance; p-n junction depth; current-voltage characteristic; photosensitivity of the original optical polychromator device [1] and solar imitator – with definition of the open-circuit voltage U_{oc} and short-circuit current I_{sc} in the diode. It has been shown that by selecting the PPI modes, it is possible to obtain highly efficient photocells with controlled electro-optical properties due to diffusion of Mn. For example, $U_{oc} = 0.48$ V, $I_{sc} = 0.35$ A in the photodiode as a result of the irradiation with 75 W/cm² and 10 s 3 pulses.

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BRANCHED ZnO MICROCRYSTALS. A SCANNING ELECTRON MICROSCOPY STUDY

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The vapor growth of ZnO microcrystals was studied using Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS). The microcrystals were grown by annealing ZnO, CuO and ammonium chloride powders. As a result, the ZnCl₂, ZnO and CuCl vapor was formed and condensed on Si substrate, which was gradually heated from room to preset temperature, selected in the range of 220 – 350 °C. The process lasted for 2 h.

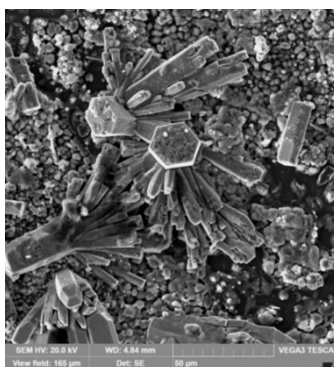


Figure 1. SEM image of branched ZnO microcrystals.

The growth proceeded in two stages. In the first stage, at ~ 240 °C, the CuCl–ZnCl₂ eutectic droplet with a low melting point was formed. With time, the droplet was oversaturated with ZnO and the solid nuclei of ZnO were precipitating from it. They served as seeds for the formation of hexagonal ZnO microrods, which were growing along the *c*-axis ([0001] direction) by the slow, thermodynamically driven Vapor–Solid mechanism. As a result, the rod-like ZnO microstructures were produced on Si substrate. The second stage of growth started when the substrate temperature was reaching 300 °C. At this temperature the secondary nucleation took place on the prism surfaces of ZnO microrods, causing the formation of branched structure (**Figure 1**). The ZnO branches were growing again along the *c*-axes, forming elongated 1D type microcrystals. In contrast to the slow growth of primer ZnO microrods, at elevated temperatures the ZnO branches were growing significantly faster. This kinetically driven process caused the vanishing of the fast growing (0001) plains, resulting in the tapering of ZnO microcrystal tips.

ZnO has a high melting point and its vapor-phase synthesis normally needs a high temperature exceeding 600 °C. The results of this work demonstrated that ZnO micro- and nanocrystals, together with branched ZnO structures, can be grown from the vapor phase at a low temperature, close to 300 °C.

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SYNTHESIS OF NANOMATERIALS FROM THE GAS MIXTURE CONTAINING NH_3 AND HCl

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The purpose of this work was to study the ability of an $\text{NH}_3 + \text{HCl}$ gaseous mixture to produce copper-based nanomaterials. A gas mixture containing both reactants can be easily produced by heating the solid powder of NH_4Cl at temperatures exceeding 340°C . The vertical quartz reactor with CuO source on its bottom was first evacuated and then heated up to 750°C . After reacting with gas mixture the volatile species were formed and condensed on the Si substrate placed in the cold zone above the CuO source. The obtained nanomaterials were analyzed by the transmission and scanning electron microscopy, X-ray diffraction and energy dispersive spectroscopy.

Nanomaterials with different shapes and compositions were synthesized depending on the Si substrate temperature, which was changed in the range of $250 - 500^\circ\text{C}$. These materials include CuO , CuCl , and CuCl_2 nanocrystals and dendrite-like structures. The most interesting synthesized nanostructures were the elongated surface nanobubbles with the average wall thickness of 80 nm and heights up to tens of micrometers. They were formed of CuCl , which is strongly hygroscopic and degrades in the atmosphere. The surface bubbles may be blown out due to the decomposition of two chemicals that are formed in the reactor, namely, Cu_2OCl_2 and CuCl_2 . The detailed thermochemical analyses of reactions led us to the conclusion that the thermal decomposition of CuCl_2 , accompanied by the release of Cl_2 , is the most probable reason for the formation of surface bubbles.

It was shown that the chemical activity of the $\text{NH}_3 + \text{HCl}$ gaseous mixture can be farther increased by introducing hydrazine (N_2H_4) vapor into the reactor, which easily decomposes to nitriding (NH , NH_2) and reducing (H_2 , atomic H) species.

This work was financially supported by the Shota Rustaveli National Science Foundation grant YS-19-087.

DEVELOPMENT OF PROMISING CATHODE MATERIALS BASED ON MODIFIED SPINELS FOR LI-ION ACCUMULATORS

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Nowadays Li-ion accumulators represent an important technology of broad interest. More over lithium rich compounds represent a promising cathode material of Li-ion accumulators due to their high electrochemical properties [1, 2]. These compounds are of great interest mostly because of the high capacity. However, a number of disadvantages, such as voltage drop caused by unwanted phase transformations during cycling, as well as low operational performances still limit their application. Improved cycling stability can be achieved by cathode materials doping (modifying). Within the framework of carried out investigations:

1. Promising cathode materials based on Fe (iron) – modified lithium manganese type spinels $\text{LiMn}_x\text{Ni}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$ (where $\text{Me} = \text{Fe}$, $x = 0.1 - 0.4$) have been developed.
2. The conditions for obtaining phase-pure, nanostructure cubic spinel samples based on Li_2CO_3 , Mn_2O_3 , Ni_2O_3 and Fe_2O_3 starting reagents have been optimized.
3. A number of solid-phase synthesis methods (700 °C) were used. Among them, the melt-saturation method ($T_1 = 180$ °C, $\tau_1 = 2.5$ h; $T_2 = 700$ °C, $\tau_2 = 5$ h) has been used. Based on modern analysis methods, it was proved that samples of the composition $\text{LiFe}_x\text{Ni}_{0.5-x}\text{Mn}_{1.5}\text{O}_4$, where $x = 0.1 - 0.4$, represent phase-pure spinel.

Cathode materials for Li-ion accumulators containing manganese, iron and nickel can be a cheap alternative to commercial Li_2MnO_4 and LiCoO_2 samples. Fe–Mn based systems are also attractive due to abundance of iron and manganese in nature.

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NANOSTRUCTURE CONTROL OF SILICIDE AND BORIDE FOR THERMAL-TO-ELECTRIC ENERGY CONVERSION

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Thermoelectric (TE) energy conversion has received renewed attention in recent years, because it has a potential to be utilized for electric power generation from waste heat. Efficiency of the energy conversion device is fundamentally limited by the properties of TE materials. The inherent efficiency of any TE materials is determined by a dimensionless parameter ZT given by $ZT = S^2 \sigma T / \kappa$, where S , σ , T and κ are the Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity, respectively. The ZT indicates that materials having lower κ and higher S and σ are desirable for TE application.

We are studying TE properties of silicide and boride, particularly β -FeSi₂ and alkaline-earth hexaboride, because they possess high Seebeck coefficient, while their thermal conductivity is rather high as compared with conventional TE materials. Reduction of the thermal conductivity is necessary to improve their TE performance. In the present study, we are trying to synthesize these silicide and boride with fine microstructure, because smaller grain increases phonon scattering at grain boundaries.

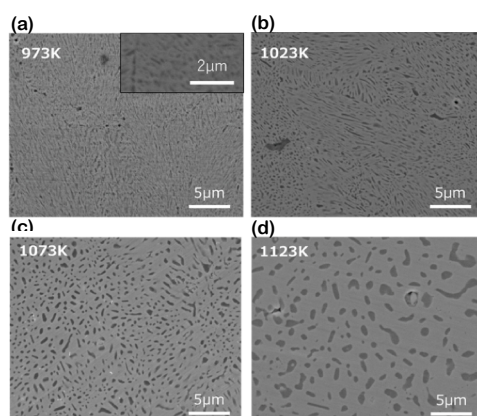


Figure 1. Microstructure of Si / β -FeSi₂ (gray matrix: β -FeSi₂, dark precipitates: Si) heat treated at (a) 973, (b) 1023, (c) 1073, and (d) 1123 K.

We synthesized Si dispersed β -FeSi₂ (Si / β -FeSi₂) by heat treatment of α -Fe₂Si₅ phase. **Figure 1** shows SEM micrographs of the Si / β -FeSi₂ obtained at various heat treatment temperatures. Size of the precipitated Si decreases down to 200 nm with decreasing heat treatment temperature, and thermal diffusivity was successfully decreased.

As for the boride, we synthesized SrB₆ fine particle by the reaction of SrCl₂ and NaBH₄ at 1073 K for 8 h in Ar atmosphere. This is low temperature process compared with borothermal reduction (conventionally 1500 K or higher). The particle size was estimated to be several tenth nm. Thermal diffusivity of a sintered body of the low temperature synthesized SrB₆ fine particle was lower than that of a specimen obtained by the borothermal reduction. These results suggest that the fine microstructure is effective to improve TE properties of silicide and boride.

MORPHOLOGICALLY DESIGNED NOVEL NANOCARBON MATERIALS DERIVED FROM HIGHLY STABLE SWCNT INKS

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Confinement of atoms, molecules, and ions in nanoscale carbon pore spaces induces unusual high pressure-compression effect. This is because graphene-like structures contain dense layers of carbon atoms, providing the strongest interaction with atoms and molecules per weight. For example, we can prepare atomically thin 1D chains of sulfur inside a single-wall carbon nanotube (SWCNT) and a double-wall carbon nanotube [1]. Synchrotron XRD provides sharp diffraction peaks coming from crystalline 1D structure of sulfur atoms. 1D sulfur inside a carbon nanotube is metallic based on Raman spectra and resistivity measurements over a wide temperature range.

Graphene exhibits high electrical conductivity. Nanoporous carbon consists of nanoscale disordered graphene units and also has a relatively high electrical conductivity. When ions are confined in the extremely narrow carbon nanopores, they induce image charges on defective carbon walls, thus reducing the ion-ion Coulomb repulsion [2]. This effect provides new insight into high-performance supercapacitors [3].

There is need for an efficient dispersant that would separate bundled SWCNTs. We have developed a Zn–Al sol–gel dispersant [4] as an alternative to widely used surfactants. The Zn–Al dispersant can be more easily removed from SWCNTs than surfactants. Then, we can uniformly deposit SWCNTs on PET [5] and flexible glass [6], resulting in a highly conductive film with transparency in the near UV region in the range of 80 – 90 % that is temperature independent up to ≈ 600 K. The thermal stability of the SWCNT film on flexible glass exceeds that of ITO [6]. Our approach provides also SWCNT inks capable of forming free-standing SWCNT films, which provide excellent support for Pt nanoparticles used in fuel cells and SWCNT nets [7].

The Zn–Al dispersant enables to prepare stress sensors based on creased SWCNTs encapsulated in polydimethylsiloxane (PDMS) with non-fluorinated water-repellant coating. The compact design and superior water resistance of the sensor, along with its appealing linear response and large stretchability, demonstrates the scalability of such sensors applications [8]. These sensors may be combined with flexible electrodes operating in aqueous environment.

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PSEUDO-PROTEIN-BASED NANOPARTICLES SHOW PROMISE AS CARRIERS FOR OPHTHALMIC DRUG DELIVERY

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Drug delivery to treat ocular diseases still is a challenge in ophthalmology [1]. One way to achieve drug delivery that is investigated currently is topical administration of drug-loaded polymeric nanoparticles (NPs) that are able to penetrate ocular barriers [2]. The purpose of this study is optimal preparation of NPs made from pseudo-proteins and evaluation of their ability to penetrate ocular tissues.

Biodegradable NPs of various types were prepared by nanoprecipitation of pseudo-protein composed of L-leucine, 1,6-hexanediol and sebacic acid (8L6). Arginine-based cationic polyester amides 8R6 and comb-like polyester amide containing lateral PEG-2000 chains along with 8L6 anchoring fragments in the backbones were used to construct positively charged and PEGylated NPs. They were loaded with fluorescein diacetate (FDA) or rhodamine 6G (Rh6G) as fluorescent probes. Suspensions of the NPs were given to cultivated microglial cells and RPE cells as well as topically on eyes of C57BL/6 mice. Penetration of NPs into the eyes was checked by fluorescence analysis.

NPs were prepared, and their properties were characterized. Cultured microglial cells and RPE cells took up the NPs. After topical administration, penetration of NPs into the cornea of the eyes could be clearly shown. Small amounts of fluorescent dyes were also found in the lens, the retina and the sclera depending on the type of NPs. The results show that the new pseudo-protein-based NPs penetrate ocular tissues after topical administration and are internalized by the cells. This raises confidence that the NPs may be useful carriers of therapeutic agents for ocular delivery.

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LASER TECHNOLOGIES OF NANOSYSTEMS PREPARATION

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The usage of laser technologies for different materials manufacturing has more than half century history when Soviet, American, Japanese and British researchers demonstrated the light sources applicable for novel materials production [1].

Toda lasers applications in material science and technology are broad and diversified. Various laser technologies have started integrating into major materials preparation processes, including laser cutting, drilling, welding, bonding, marking, patterning, measurement, deposition, etc.

Drivers of laser methods differ from one process step to another. However, there are similar and common drivers for applicability of lasers to nanosized structures processing and the choice of the most suitable laser technology type strongly depends on material to be processed, processing parameters, and the manufacturing process step.

Laser type is defined by parameters such as wavelength, emitting UV, green, or IR light, as well as the duration of pulse, for example nanosecond, picosecond or femtosecond. Users must consider which pulse length and wavelength is right for their semiconductor-semimetal-insulator process step and application. Excimer lasers are widely used in numerous fields of scientific research and technology, both as primary sources and, as pump sources for tunable dye lasers. These lasers are also commonly used in pulsed laser deposition systems, where their large flux, short wavelength and non-continuous beam properties make them ideal for preparation of a wide range of materials.

One of the green methods for preparation of metal nanoparticles is laser ablation technique that offers a unique tool for nanofabrication of nanoparticles. In this technique, the high-power laser ablates the metal plate and the nanoparticles are formed in the liquid. The important parameters to produce the metal nanoparticles are energy, wavelength, repetition rate of laser, ablation time, and absorption of an aqueous solution [2].

The most suitable and prospective method for preparation of nanosystems having different origin – from elementary nanoparticles to nanostructured compounds is laser plasma deposition technology. The properties of nanomaterials prepared by laser plasma technic are unique, and they are not reproducible by any other method including chemical ones [3].

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MAGNETOEXCITONS IN NOVEL TWO-DIMENSIONAL MATERIALS IN MONOLAYERS, BILAYER, AND VAN DER WAALS HETEROSTRUCTURES

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In this talk, we review and provide new development in the theory of Rydberg states of direct and indirect magnetoexcitons in novel two-dimensional materials: transition-metal dichalcogenides (TMDC), Xenes (silicene, germanene, and stanene), and phosphorene. The direct magnetoexcitons are considered in freestanding and encapsulated by hBN monolayers of 2D materials. Indirect magnetoexcitons are considered in the bilayer and van der Waals heterostructures formed by two layers of 2D materials separated by a few hBN monolayers. The systems are considered in presence of the external magnetic field perpendicular to the system.

We present calculations and review of binding energies and diamagnetic coefficients (DMCs) of magnetoexcitons of the Rydberg states: $1s$, $2s$, $3s$, and $4s$, obtained by numerical integration of the Schrödinger equation using Rytova–Keldysh potential [1, 2] for direct magnetoexciton and both Rytova-Keldysh and Coulomb potentials for indirect magnetoexcitons. The latter is done to study the role of screening in novel 2D materials when a two-body problem in restricted 3D space is considered.

In the case of Xenes, the monolayers and heterostructures are in presence of parallel magnetic and electric fields, which are perpendicular to the structures [3]. We present our result for direct magnetoexcitons in TMDC monolayers [4] and indirect magnetoexcitons in the bilayer and the double-layer TMDC heterostructures [5]. Our study is extended to magnetoexcitons in phosphorene monolayers and heterostructures which are different from other 2D semiconductors, due to their high anisotropy of the dispersion relations for the charge carriers and different exciton-hole masses along zig-zag and armchair directions.

We demonstrate that the binding energies of direct and indirect magnetoexcitons in Xenes, TMDCs, and phosphorene monolayers and heterostructures can be tuned by applying an external magnetic field. For magnetoexcitons in Xenes, the external perpendicular electric field allows to tune electron and hole masses and, therefore, gives an additional knob to tune binding energies and DMCs. Moreover, in van der Waals heterostructure the number of hBN layers that separate monolayer serves as an additional degree of freedom that can be used to tune indirect magnetoexcitons binding energies and DMCs.

Our calculations show that the choice of the interaction potentials has significant effect on the binding energies of indirect magnetoexcitons and diamagnetic coefficients. The outlined ways to tune binding energies and DMCs of direct and indirect magnetoexcitons in Xenes, TMDCs, and phosphorene monolayers and heterostructures give the possibility of electronic devices design that can be controlled by the external electric and magnetic fields and the number of hBN layers.

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STUDY OF GOLD THIN FILMS OBTAINED BY DIFFERENT TECHNOLOGICAL MODES

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Research has been conducted to optimize a mercury sensitive sensor [1]. The stability of the mercury-sensitive element is determined by the perfection of the film structure. The films obtained by condensation are highly dispersed unstable systems whose stability changes during formation. Therefore, in order to get a complete picture of the formation of the all stages of the growth of the film, from its conception to its complete formation, were considered as much as possible.

The studies were performed using conventional and permeable electron microscopy. Thin gold strips coated on the polished sapphire and NaCl crystals were used for the studies by thermal evaporation in vacuum and magnetron scattering. Tapes with thicknesses of 20, 40, 100 and 200 nm were studied (these thicknesses are of interest in our study). If the coating temperature is low (in our case 25 °C) the structure of the thin film does not change with increasing film thickness (up to 500 nm) and is a complex structure without any orientation of the polycrystalline.

The situation changes with increasing of temperature basal body. Experiments were performed at 50 ° intervals when the diaphragm temperature changed. It was found that with increasing the temperature of the basal body, the structure of the film were adjusted. It lasts up to 400 – 450 °C. With further increase in temperature the order is again disturbed (**Figure 1**).

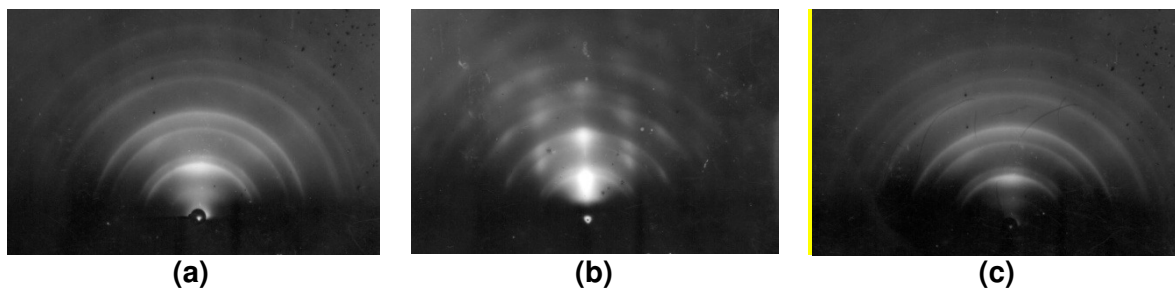


Figure 1. Electronograms of 100 nm thick gold strips deposited on a sapphire plate at different temperatures: **(a)** 20, **(b)** 300, and **(c)** 500 °C.

During the study, already formed films were annealed at different temperatures. It was found that annealing films has a positive effect on the structure of the films. In particular, it was found that the best results are obtained by annealing the films for 30 min at 350 – 400 °C.

It was found that for our particular case it is optimal to lay gold thin films (20 – 100 nm) at a temperature of 300 – 350 °C and further anneal for 30 min at 350 – 400 °C.

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GREENER SYNTHESIS OF CHEMICAL COMPOUNDS AND MATERIALS

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Modern trends in the greener synthesis and fabrication of inorganic, organic and coordination compounds, materials, nanomaterials, hybrids and nanocomposites are discussed. Green chemistry deals with synthesis procedures according to its classic 12 principles, contributing to the sustainability of chemical processes, energy savings, lesser toxicity of reagents and final products, lesser damage to the environment and human health, decreasing the risk of global overheating, and more rational use of natural resources and agricultural wastes.

Greener techniques have been applied to synthesize both well-known chemical compounds by more sustainable routes and completely new materials. A range of nanosized materials and composites can be produced by greener routes, including nanoparticles of metals, non-metals, their oxides and salts, aerogels or quantum dots.

At the same time, such classic materials can be improved or obtained by cleaner processes as cement, ceramics, adsorbents, polymers, bioplastics and biocomposites. Several non-contaminating physical methods as microwave heating, ultrasound-assisted and hydrothermal processes or ball milling, frequently in combination with the use of natural precursors, are of major importance in the greener synthesis, as well as solventless and biosynthesis techniques. Non-hazardous solvents including ionic liquids, use of plant extracts, fungi, yeasts, bacteria and virus are also discussed in relation with materials fabrication.

Availability, necessity and profitability of scaling up green processes are discussed.

EFFICIENT AND CONTINUOUS GENERATION OF ELECTRICITY FROM TRIBOELECTRIC NANOGENERATORS OPERATED IN THE CONTACT-SEPARATION MODE BY A SCOTCH YOKE SYSTEM

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Triboelectric nanogenerators (TENGs) obtains electricity from renewable mechanical energy sources such as everyday human activities, wind and waves. Thus, TENG technology is environment-friendly and it contributes to sustainability of nature and human society. TENGs show excellent efficiency at low frequencies around 5 Hz which are best for energy sources mentioned above [1]. TENGs generate electricity by contact electrification between two materials and the stored electrostatic energy. Thus, in order to harvest more energy by TENGs, contact area should be large and an appropriate material pair should be selected.

For this study, TENGs are fabricated with AgNW electrodes with a large surface to volume ratio thus contact area of triboelectric materials with electrodes increases and more charges gather on the surface of the electrodes. For fabrication of TENGs, AgNWs are synthesized by a simple polyol method described elsewhere [2]. Then, AgNWs are deposited onto substrates by spray-coating. TENGs are fabricated as two polymer films which are dip-coated over prepared AgNW electrodes are faced each other with a small gap as shown in **Figure 1a**.

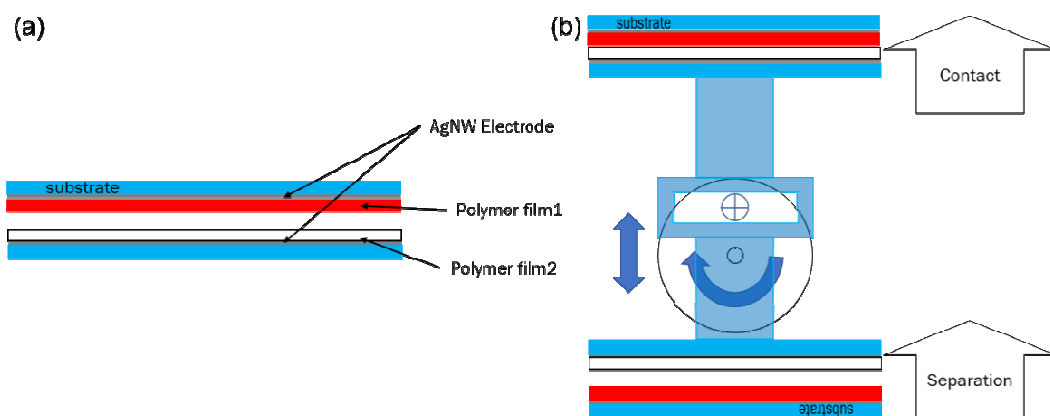


Figure 1. (a) structure of TENG and (b) operation of TENG by scotch yoke system.

And for application, TENGs are operated in the contact-separation mode. A scotch yoke is used to switch the rotational motion into the linear motion for contact and separation of TENGs as shown in **Figure 1b**. TENGs continuously generate electricity by rotational motions.

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THERMOELECTRIC PROPERTIES OF LAYERED CALCIUM COBALTITE DOPED BY PARTICLES OF COBALT, COPPER, AND THEIR OXIDES

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Layered nanostructured calcium cobaltite ($\text{Ca}_3\text{Co}_4\text{O}_{9+\delta}$) is prospective oxide thermoelectric for high-temperature applications, and its thermoelectric performance may be essentially improved, particularly, via doping by micro- and nanoparticles of semiconductors (B_4C , TiC), metal oxides (ZrO_2 , CaZrO_3) or noble metals (Ag , Au) [1, 2]. In this work the results of attempt of enhancing of thermoelectric properties of $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta}$ through doping by particles of transition metals (Co , Cu), and their oxides (Co_2O_3 , Co_3O_4 , Cu_2O , CuO) are presented.

Ceramic samples of layered calcium cobaltite with different dopants (see above) were prepared using ceramic method and sintered at different conditions at temperatures below and above of temperature of peritectoid decomposition of $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta}$ ($T_p = 926^\circ\text{C}$ in air) and their electrical conductivity (σ) and thermo-EMF (S) were measured within $25 - 825^\circ\text{C}$. Effect of nature of dopants and their content in composites, as well as thermal prehistory of the samples on their phase composition, microstructure, porosity, electrotransport (σ and S) and thermoelectric properties (power factor (P), $P = S^2\sigma$) was analyzed.

All the prepared materials were p-type semiconductors like parent layered calcium cobaltite. It had been found that σ values of ceramics are enhanced at increasing of sintering temperature of the samples which is due to the decreasing of their porosity. Thermo-EMF coefficient values of obtained materials increases at creation in them phase inhomogeneity and this is more pronounced when role of dopant among oxides plays Co_2O_3 , and copper oxides (Cu_2O and CuO). So, porosity of $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta}$ ceramics sintered at $T > T_p$ decreases more than 2 times comparing to the ceramics sintered at common conditions ($T < T_p$) which results in appropriate increasing of its σ and P values: ≈ 300 and $140 \mu\text{W}/\text{m}\cdot\text{K}^2$ at 775°C . Values of power factor of ceramics having $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta} + 8 \text{ mas. \% } \text{Co}_2\text{O}_3$ and $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta} + 8 \text{ mas. \% } \text{Cu}_2\text{O}$ sintered at $T < T_p$ are equal ≈ 220 and $210 \mu\text{W}/\text{m}\cdot\text{K}^2$ respectively at 775°C which is about 1.5 time larger than for parent $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta}$ cobaltite.

Our results demonstrate that using unexpensive additives and varying thermal prehistory of ceramics based on the layered calcium cobaltite one can essentially improve its thermoelectric performance. That may be used for development of new high-temperature oxide thermoelectrics based on $\text{Ca}_3\text{Co}_4\text{O}_{9+\delta}$ which will be prospective for effective conversion of high-temperature heat into electrical energy.

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CONVENIENT WAY FROM METAL COMPLEXES TO NANOSIZE METAL OXIDES

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Nanosized mixed-metal-oxide catalysts are widely used in various industrially relevant processes like Fischer–Tropsch synthesis, CO or NO_x removal from gases. Transition metal ions like Ag, Co, Cr and Fe coordinated with reducing ligands as NH₃, pyridine or urea and salts with oxometalate anions (MnO₄⁻, CrO₄²⁻, Cr₂O₇²⁻) are used to prepare nano-sized mixed spinel-type metal-oxides with planned composition, properties, and structure.

The utilization fields of the formed mixed oxide catalyst are determined by the distribution of the cationic and anionic metals in various valence states in crystallographic positions (T-4 and OC-6) of the formed spinels. The methods are used for the synthesis of mixed metal-oxides do not allow the control of these properties, because they include steps at high temperatures when the mobility of atoms leads to the formation of the thermodynamically stable structures, characterized by its favored distribution of metal atoms among positions and valence states. The unique feature of the catalyst synthesis method developed by us [1 – 4] is based on the controlled thermal decomposition of tetraoxometalates of transition metal ions coordinated by reducible ligands at relatively low temperatures (80 – 180 °C), releasing gas-phase products formed from the ligands and leave back an amorphous highly defectuous mixed oxide precursor. This is a solid-phase reaction, which forms mixed oxides with metastable structures because at the low temperature used, the metal ions remain in the crystallographic positions of the precursor salt. For example, hexaquaairon (III) permanganate results (Fe,Mn)O type and (Fe,Mn)₃O₄ type mixed oxides depending on the atmosphere and temperature of decomposition. The original spinel structures in some cases can be oxidized into defect-spinel structures and finally to (Fe,X)₂O₃ type oxides.

It was observed in the case of hexaureairon (III) permanganate. Our method enables one to set the ratio of the metal ions arbitrarily by starting from an isomorphous solid solution in which we partially replaced the metal ion by another one and / or the anion by another tetraoxometalate or by an “innocent” anion (which forms gaseous products due to the lack of metal atoms, e.g., MnO₄⁻ by ClO₄⁻). For example, the hexaureairon (III) salts can be co-crystallized with various trivalent metal (e.g., chromium, cobalt, aluminum or gallium) urea complexes with the same or similar anions (ClO₄, MnO₄, ReO₄, CrO₄, SO₄, SeO₄). In this way, e.g., the [(Fe_{0.5}Cr_{0.5})(urea)₆](MnO₄)_{0.5}(ClO₄)_{2.5} gave (Fe, Cr, Mn) oxide precursor with Fe : Cr : Mn = 1 : 1 : 1 overall ratio. Due to a large number of crystal defects, nanocrystallites are formed, both being favorable for catalysis.

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PHOSPHORENE AND ARSENENE PRODUCTION FOR CATALYSIS, SENSING AND ENERGY STORAGE

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Layered phosphorus P (phosphorene) and arsenic As (arsenene) are novel promising materials of 2D crystals family (pnictogen group) which have widely attracted the researchers' interest ranging from (opto)electronics [1], energy storage [2], catalysis [3] to (bio)sensing [4] and healthcare technologies [5]. The exotic nature of P and As monolayers consists of their anisotropic atomic arrangement and possesses attractive properties such as high thermoelectric potential, configurable optical properties, a wide band-gap tunability (0.1 – 1.8 eV) and, therefore, adjustable electronic properties. However, innovation surrounding novel quantitative and scalable way of the synthesis of (mono-)few-layer phosphorene (FP) and arsenene (FA) has faced an outstanding challenge due to the process irreproducibility and environmental degradation ability of the materials and, moreover, the lack of experimental results on arsenic. Nowadays beginning with the production of pnictogens, electrochemical exfoliation has been found as an extremely effective method for the preparation of 2D materials from their bulk form [6].

Herein we report low-potential anhydrous electrochemistry as an extremely effective method for the preparation of high-quality FP and FA in a high yield. A variety of analytical methods has revealed high-quality phosphorene and arsenene of 1 – 5 layers with good crystallinity and micrometer lateral sizes. We discuss the great promise of FP- and FA-based catalysts for hydrogen evolution, oxygen evolution and oxygen reduction reactions as well as show performance of FP- and FA-enabled electrodes for complex monitoring of volatile organic compounds and energy storage devices. We anticipate, proposed electrochemistry route towards FP and FA will broaden the materials' scope applications in new-generation devices.

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PREPARATION AND PROPERTIES OF COMPLEXES BASED ON PECTIN–Ag NANOCOMPOSITES AND KANAMYCIN

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Antibiotic resistance is one of the biggest threats to global health and food security today. One of the promising approaches to overcome bacterial resistance is the use of metallic nanoparticles [1], for example, silver nanoparticles (AgNPs). Another effective way to prevent and control the spread of antibiotic resistance is combining silver nanoparticles with antibiotics. These combinations are able to synergistically inhibit bacterial growth [2]. The aim of this work was to obtain complexes of AgNPs with kanamycin (KAN).

Pectin–Ag nanocomposites, which are AgNPs stabilized by a pectin shell, were synthesized by “green chemistry” method [3], using pectins with different degrees of esterification and amidation. It was shown that the ζ -potential value of AgNPs decreases in $\sim 1.7 - 2.2$ times upon addition of KAN to pectin–Ag nanocomposites and is equal to $-(21.7 - 25.5)$ mV. Furthermore, the increase of hydrodynamic diameter of AgNPs compared with initial one in $\sim 1.2 - 1.4$ times (from 284.8 – 649.2 to 384.2 – 773.8 nm) was observed. It was found that percentage of KAN binding to pectin–Ag nanocomposites varies from 16 to 68 % and depends on the type of pectin (Figure 1). The structure of obtained complexes was studied by FTIR spectroscopy.

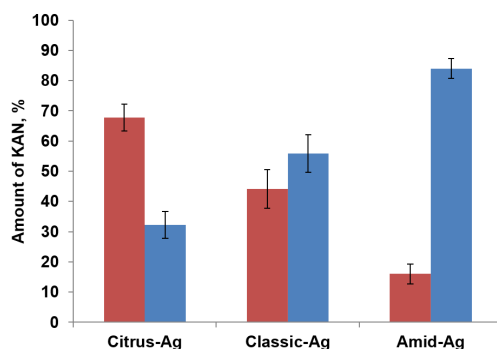


Figure 1. Binding of KAN to pectin–Ag: red section – bound KAN and blue section – native KAN.

The pectin–Ag nanocomposites and obtained pectin–Ag / KAN complexes were used for fabrication of solvent-cast thin films with antibacterial activity.

The work was financially supported by SCST of the Republic of Belarus (project X19INDG-002).

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THERMOELECTRIC MATERIALS BASED ON THE LAYERED SODIUM COBALTITE

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The nanostructured layered sodium cobaltite (LSC) Na_xCoO_2 is perspective basis for development of materials of sodium ion battery (SIB) electrodes and *p*-branches of high-temperature thermoelectric generators. The physicochemical and functional characteristics of the layered sodium cobaltite can be improved by varying its cationic composition, and therefore research of derivatives of this phase is of considerable interest.

We have prepared by means of the solid-state reactions method a wide range of LSC derivatives with different sodium content and partial substitution of cobalt with transition and heavy metals. Their crystal structure and microstructure, electrical transport (electrical conductivity (σ), thermo-EMF (S)), thermophysical (thermal expansion, thermal diffusivity (η), thermal conductivity (λ)) properties in the range 300 – 1100 K were studied. The values of the power factor (P) and thermoelectric figure of merit (ZT) of LSC were calculated using formulas $P = S^2 \cdot \sigma$ and $ZT = PT/\lambda$. The lattice (λ_{lat}) and electronic (λ_{el}) contributions to the thermal conductivity were found using relationship $\lambda = \lambda_{\text{el}} + \lambda_{\text{lat}}$, $\lambda_{\text{el}} = \sigma LT$, where L is the Lorentz number ($L = 2.45 \cdot 10^{-8} \text{ W}\Omega\text{K}^{-2}$).

Effect of sodium content, nature of substituting cobalt metal and substitution degree on the crystal structure, microstructure, chemical stability in atmosphere containing water vapors and carbon dioxide, physicochemical and functional properties of LSC derivatives was analyzed. It was shown, that variation of cationic composition of LSC allows to obtain thermoelectric ceramics with improved characteristics [1 – 3]. For example, the power factor values of $\text{Na}_{0.89}\text{CoO}_2$, $\text{Na}_{0.55}\text{Co}_{0.90}\text{Cr}_{0.10}\text{O}_2$, $\text{Na}_{0.89}\text{Co}_{0.90}\text{Ni}_{0.10}\text{O}_2$ and $\text{Na}_{0.55}\text{Co}_{0.90}\text{Bi}_{0.10}\text{O}_2$ cobaltites at 1100 K are respectively 829, 917, 919 and 1018 $\mu\text{W}/\text{m}\cdot\text{K}^2$. The values of the dimensionless thermoelectric quality index for cobaltites $\text{Na}_{0.89}\text{Co}_{0.90}\text{Bi}_{0.10}\text{O}_2$, $\text{Na}_{0.89}\text{Co}_{0.90}\text{Ni}_{0.10}\text{O}_2$, $\text{Na}_{0.55}\text{Co}_{0.90}\text{Sc}_{0.10}\text{O}_2$ and $\text{Na}_{0.89}\text{CoO}_2$ at 1100 K are 0.83, 1.12, 1.45 and 1.57 respectively. This value exceeds the theoretical criterion ($ZT > 1$) that determines materials of practical interest for thermoelectric conversion, and suggests that LSC is a potentially attractive material for thermoelectric conversion.

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THE PROBLEM OF INTERDEPENDENCE OF ALGAE *Spirulina platensis* AND pH

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In the given work an attempt has been made to determine the problem of interdependence of cyanobacterium *Spirulina platensis* and pH.

For this purpose we considered some cases, when during the first days of experiment the following chemical elements: Cu, Zn, Ni, Hg, Cd and Ag were introduced separately into nutrient medium Zarrouk of the mentioned algae with different amount and at different time.

The results were obtained by the method of atomic absorption spectrometry and were given in the form of tables.

LAYER-BY-LAYER BUILDUP OF ULTRATHIN FILMS BASED ON CHITOSAN, PECTIN AND THEIR NANOCOMPOSITES WITH SILVER NANOPARTICLES

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The polyelectrolyte multilayer films can be used for altering surface properties and they are of great interest for biomedical applications [1]. The aim of this study was to investigate the quantitative regularities of formation of multilayer films based on pectin (Pect), chitosan (Chit) or their nanocomposites with Ag nanoparticles. Nanocomposites pectin–Ag (Pect–Ag) and chitosan–Ag (Chit–Ag) were synthesized by “green” chemistry technique [2]. Multilayer films were prepared by alternating adsorption of the oppositely charged components from their solutions and quantitative regularities of film formation were assessed by quartz crystal microbalance with dissipation monitoring.

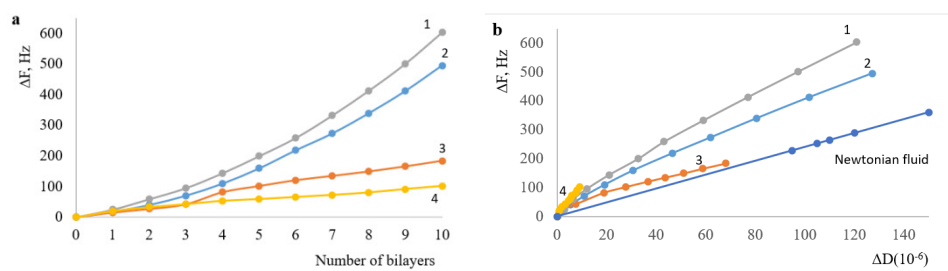


Figure 1. Frequency shift upon alternating adsorption of components (a) and frequency shift versus dissipation shift (b) during LbL films formation: (Chit–Ag / Pect)₁₀ (1), (Chit/Pect)₁₀ (2), (Chit/Pect–Ag)₁₀ (3) and (Chit–Ag/Pect–Ag)₁₀ (4).

It has been shown that the dependence of resonator frequency shift (ΔF) on the number of bilayers was linear and exponential upon using Pect–Ag and Pect as polyanion component of multilayer systems respectively (Figure 1a). The film thickness increased in 5.4 times (from 16.8 ± 2.6 to 90.9 ± 9.5 nm) in the following range: (Chit–Ag / Pect–Ag)₁₀ – (Chit / Pect–Ag)₁₀ – (Chit / Pect)₁₀ – (Chit–Ag / Pect)₁₀. The elasticity of prepared films enhanced in the range (Chit / Pect–Ag)₁₀ – (Chit / Pect)₁₀ – (Chit–Ag / Pect)₁₀ – (Chit–Ag / Pect–Ag)₁₀ (Figure 1b), while their shear modulus increased by 3.2 times (from 143 ± 7 to 462 ± 83 kPa).

This study was financially supported by State Committee on Science and Technology of the Republic of Belarus (project X19INDG-002).

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NANOCOMPOSITE HYDROGELS AND ITS APPLICATION FOR ENVIRONMENTAL REMEDIATION

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One of the extremely major problem facing the modern world is the shortage of natural resources and the environmental pollution resultant from industrial activities. It is no doubt that water is an important natural resource and it needs protection. Although, several physical, chemical and biological treatment methods have been developed and successfully adopted in to the industry to solve this problem, in recent years, adsorption technique has been re-gaining interest due to its advantages on the removal of stable pollutants, flexible process design and process economy. In adsorption, one of the key parameter that influence treatment recovery is the adsorbent material. Therefore, adsorbent materials are of great scientific and technological interest owing to their ability to interact with specific substances and efficiently separate them from a mixture.

Over the last years, nanotechnologies have been implemented in almost all branches of human live. Until now, numerous nanomaterials have produced and used to eliminate inorganic and organic species from wastewater effluents, in many cases, it was found more efficient than the conventional adsorbents. Within this group, hydrogels which consisted a group of polymeric materials has received high interest due to the several advantages. The hydrophilic structure of which renders them capable of holding large amounts of water in their three-dimensional networks. Extensive employment of these products in a number of industrial and environmental areas of application has considered to be of prime importance [1].

However, relatively lower mechanical properties, required a long time to reach a saturated state and difficulties associated with the regeneration and disposal are the main obstacles for their practical application. Therefore recently, some attempts have been performed to made them more functional (well-defined porosities, more controllable surface properties) by the incorporation of nano- or micro-particles of inorganic materials, such as clay minerals graphene oxide, iron oxide CNT, etc. into the polymer networks [2].

In this article, the fundamental concepts, classification, physical and chemical characteristics, production methods and technical feasibility of their utilization was reviewed base on the composite hydrogel. A special attention has given to utilization of them for wastewater purification especially for the effluent received from textile industry.

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ULTRA-FAST SINGLE-PHOTON DETECTORS IN THE NEAR FUTURE

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Single photon detectors capable to determine the photon energy and to provide high count rates are demanded in quantum electronics, astrophysics, high energy physics, quantum informatics, telecommunication systems, quantum metrology, measuring systems for applications in medicine, homeland security and other fields [1]. Among the developments of last 18 years, superconducting nanowire single-photon detectors are considered as the most promising. According to their characteristics, they are more favorable in comparison to all earlier known detectors. They possess low dark-count rate, gigahertz count rate and are able to register photons in a wide range of the electromagnetic spectrum [2]. The thermoelectric single-photon detector is capable of exhibiting similar characteristics. According to theoretical estimation they can compete with superconducting detectors due to several advantages, in particular, a simpler design of the detection pixel and absence of strict requirements for operating temperatures [3].

In this work we have proposed a different design of the detection pixel of the thermoelectric single-photon detector. Modeling and simulation are used to study the processes of heat propagation in a four-layer detection pixel of the thermoelectric single-photon detector after one or many photons absorption. Calculations were carried out on the basis of the equation of heat propagation from a limited volume using the three-dimensional matrix method for differential equations. The temporal dependence of the amplitude of the signal appearing on the detection pixel was calculated for different designs of the detection pixel, different energies of photons absorbed in different areas of the detection pixel. It is shown that a single-photon thermoelectric detector will have terahertz count rate, high energy resolution from IR to UV, and detection efficiency exceeding 90%. Detectors with such characteristics are in demand in various fields of science and may have a wide range of practical applications in future technologies.

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SINGLE-PHOTON THERMOELECTRIC DETECTOR WITH Bi(Pb)-2223 SUPERCONDUCTING THIN FILM LAYERS

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Single-photon detectors capable to register the photon energy and provide high counting rates are in demand in many areas. Computer simulation of heat propagation processes in a detection pixel of thermoelectric single-photon detector (TSPD) has shown that they can have high count rate and energy resolution. In our early work we have shown that a three-layer detection pixel of TSPD, in which (La,Ce)B₆ or CeB₆ hexaboride is used as the thermoelectric layer, and Nb, Pb or YBCO superconductors serve as the absorber and heat sink, can register single photons in a wide range of electromagnetic spectrum from IR to X-ray, providing an energy resolution of not less than 1% and the counting rate of more than tens of GHz [1]. However, the most important characteristic of single-photon detectors is the detection efficiency, namely, the ratio of the number of registered photons to the number of photons hitting the detector.

We present the results of computer simulation of heat propagation processes in the three- and four-layer detection pixel of TSPD after the absorption of 1–1000 eV energy photons. The different geometries of the detection pixel consisting of SiO₂ antireflective layer, CeB₆ or FeSb₂ thermoelectric sensor, absorber and heat sink of Bi(Pb)-2223 superconductor are considered. The computations based on the heat conduction equation from the limited volume are carried out by the three-dimensional matrix method for differential equations. It is shown that changing the construction of the detection pixel we can obtain a detector registering the photons in the spectral range from IR to X-ray with required energy resolution, detection efficiency and counting rate. Such a detector has a number of advantages that allow one to consider the thermoelectric detector as a real alternative to the most promising single photon detectors.

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EFFECT OF BN ADDITIVE ON THERMOELECTRIC PROPERTIES OF $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y$ CERAMICS

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In this work, boron nitride-added thermoelectric materials with nominal composition $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y(\text{BN})_x$, $x = 0, 0.10, 0.15, 0.20$, and 0.25 ($0, 0.30, 0.45, 0.60$, and 0.75 wt. %, respectively) were prepared through the solid-state reaction method.

Firstly, raw materials Bi_2O_3 , SrCO_3 , Co_3O_4 , and BN were calcined at $1040 - 1080$ K for 20 h with an intermediate manual grindings and ball milling in a planetary mill. Secondly, the resulting powder mixtures were cold isostatically pressed into pellets with 15 mm in diameter at a hydrostatic pressure of 200 MPa. Then the pellets were sintered at 830°C for 25 h in air. The temperature dependence of Seebeck coefficient and resistivity of bar-shaped samples with dimensions of $\sim 14 \times 7 \times 3.5 \text{ mm}^3$ were investigated at $T = 300 - 950$ K by a setup designed in the laboratory using a Keithley DMM 6500 multimeter. Thermal conductivity in the temperature range from 300 to 570 K was measured by the Hot Disk TPS 500 Thermal Constants Analyzer (Sweden / Canada).

Addition of boron nitride (0.60 wt. %) to $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y$ thermoelectric ceramics leads to the marked (2.9 – 1.9-fold) decrease of electrical resistivity in the temperature range from 300 to 950 K, respectively, while not affecting the Seebeck coefficient. Thermal conductivity of 0.60 wt. % BN-added $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y$ thermoelectrics increases about 2.2-fold compared to a reference (un-doped) sample in the whole temperature range under investigation (300 to 570 K). Based on obtained results, the values of power factor (PF) and thermoelectric figure of merit (ZT) were calculated. Addition of BN leads to the increase of power factor at 970 K from $0.026 \text{ mW/m}\cdot\text{K}^2$ for the reference sample to the highest value of $0.04 \text{ mW/m}\cdot\text{K}^2$ in the sample with 0.60 wt. % BN. The figure of merit ZT for $\text{Bi}_2\text{Sr}_2\text{Co}_{1.8}\text{O}_y$ thermoelectrics increases slightly with the addition of 0.60 wt. % BN from 0.0065 and 0.0170 to 0.0083 and 0.0180 at 300 and 600 K, respectively.

This work was supported by Shota Rustaveli National Science Foundation (SRNSF): FR-18-4976 / Tuning the functional properties of Co-based thermoelectrics via doping and high-energy ball milling.

GENERAL CHARACTERISTICS OF NANOPARTICLES FORMED IN IRON-BASED SYSTEMS AND PERSPECTIVES THEIR BIOMEDICAL APPLICATION

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Nowadays the magnetic nanopowders are widely used for various functional materials creation for technical and bio-medical applications that are characterized by unique magnetic, optical, and catalytic properties. Well known that the main problems for practical usage of ferrimagnetic nanoparticles in bio-medicine lies in the obtaining of homogenous powders and sols and their stabilisation against the following oxidation, phase transformation as well as development of new simple one-pot synthesis methods.

The application of the rotation-corrosion dispergation (RCD) process performed in the open-air systems based on steel or iron permits to obtain various modifications ferric oxides, transition 3d-metal spinel ferrites and core & shell type composites composed by a ferrimagnetic cores and precious metal shells [1]. To control physical-chemical parameters of the nanoparticles (phase and chemical composition, morphology and size, their magnetic and electro-kinetic properties) we chose the following parameters: the chemical composition of the dispersion medium and its pH value, red-ox condition in the system, synthesis temperature and duration of the phase formation process etc. But free oxidant entrance into the system provides the oxidative processes and formation of ferric oxyhydroxides – lepidocrocite and goethite, as additional mineral phases. Hence, the optimal RCD conditions search to form of homogenous dispersions of iron oxides, spinel ferrites, and core & shell type nanocomposites may open the ways for their practical application for technical and bio-medical aims.

In general, the phase formation process carried out under the RCD conditions is determined by the nucleation and development of the primary Fe(II)-Fe(III) layered double hydroxide (LDH) phases that play role as nanoreactors [2]. The next transformation Fe(II)-Fe(III) LDHs in water medium may run out by two ways: as solid-state transformation or dissolution-re-precipitation. At the same time when various chemical species are added in the water media their dissolved forms can interact with dissolved ferric and ferrous species and can precipitate as a new mineral phase. Heavy and precious metal cations of the solutions may be included in the crystal lattice of newly-formed nanomagnetite. In addition, the noble metals may be reduced on nanomagnetite surface and form the metal shells on ferromagnetic particles (cores).

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ELECTROLUMINESCENCE IN MOLECULAR PHOTODIODE WITH APPLIED GATE POTENTIAL

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Molecular photodiode is a nanoscale structure consisting of a fluorophore that is placed in between two metal electrodes (1M2-system). In such a system the energy of electrons transported within it, can be converted to the energy of quantum of light under certain conditions. Essentially this process is the same that occurs in organic LEDs. The difference is that due to the formation of plasmons in the nanoscale region where radiation occurs, the radiation of the fluorophore molecule is enhanced. Another important difference is that the efficiency of electroluminescence strongly depends on the kinetics of electron transitions between the neutral and charged states of the molecule [1, 2].

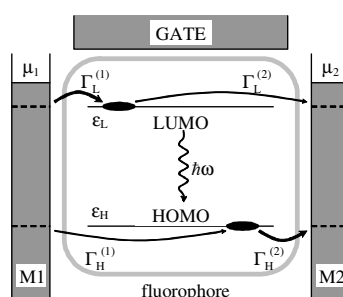


Figure 1.

We used nonequilibrium density matrix approach to describe this phenomenon. The **Figure 1** shows the scheme of formation of electroluminescence at positive polarity bias applied to the electrodes M_1 and M_2 , voltage bias $V = (\mu_1 - \mu_2) / |e|$ (μ_1 and μ_2 are chemical potentials, $|e|$ is the electron's absolute charge) under conditions where the electron jump rate $\Gamma_L^{(1)}$ from M_1 to the LUMO exceeds the rate $\Gamma_L^{(2)}$ of the transition from LUMO to the unoccupied M_2 level. In addition, in the same asymmetric photochromic molecule, the rate $\Gamma_H^{(2)}$ of the electron transition from a double-populated HOMO to M_2 is believed to exceed the rate of $\Gamma_H^{(1)}$ electron flow from M_1 to a single-populated HOMO. In this transmission mode, the probability of the P^* excited state of the molecule is the highest. Therefore, the electroluminescence power, $W \sim P^*$ is maximal.

As a result, if the electric energy $|e|V$ exceeds the HOMO–LUMO gap $\varepsilon_L - \varepsilon_H$, a stable photoactive state of the fluorophore occurs. This state proceed to the ground state with the emission of the quantum of light with frequency $\hbar\omega = \varepsilon_L - \varepsilon_H$, and then is reduced due to the transition of an electron from HOMO to M_2 and another electron from M_1 to LUMO. We have shown that, although the potential of the gate (V_g) has little effect on the HOMO–LUMO gap size, it changes the charge states of the molecule [3]. These states, as well as charge-neutral ones, are involved in the kinetics of transitions and thus are responsible for the formation of the photoexcited state of fluorophore. As a consequence, turning on the gate potential can change the quantum yield of electroluminescence by an order of magnitude.

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BORON CARBIDE AND NITRIDE NANOPARTICLES AS ^{10}B -ISOTOPE DELIVERING AGENTS IN BORON-NEUTRON-CAPTURE-THERAPY

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Role of boron-neutron-capture-therapy (BNCT) in modern radiation medicine rapidly increases [1]. In this regard, one of the main problems is achieving in target tumor the neutron-capturing boron ^{10}B isotopes concentration level needed for successful realization of the BNCT. In last decade, for this purpose there are suggested nanoparticles of various boron compounds – e.g. see the recently report on nano boron carbide B_4C [2].

There are developed two different methods of obtaining iron Fe-doped nanocrystalline boron nitride in hexagonal structure (h-BN) [3]. First method is a single technological cycle, in which the starting components are sodium tetraborate, carbamide and iron chloride. Their aqueous solution is sprayed on the heated quartz substrate and the resulting powder is first annealed in ammonia and then in hydrogen atmosphere. Second method involves the use of a suspension of already formed nanocrystalline boron nitride and water-soluble iron salts, their homogenization, dehydration, and reduction of iron by thermal treatment of the resulting mass first in air and then in hydrogen flow.

We will analyze possibilities of using the nanopowdered B_4C and h-BN:Fe as effective drug delivery agents in the BNCT.

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ELECTROMAGNETIC RESPONSE OF NANOCARBON FILMS AND STRUCTURES IN GIGA- AND TERAHERTZ FREQUENCY RANGES

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We consider electromagnetic response of nano-structured carbon films in giga- and terahertz frequency range. Thin films comprising graphene and graphene / polymer structures, carbon nanotubes and carbon nanotube / WS_2 nanotube hybrids, pyrolytic carbon, etc. are discussed as actual or potential materials for diverse electromagnetic applications: for instance to fabricate emitters, detectors, absorbers, antennas and interconnects. We investigate the main phenomena to be controlled in view of the above applications: conductivity, plasmon resonances, screening, and absorption properties, etc. and demonstrate their essential peculiarities as compared to traditional electromagnetic materials.

STRUCTURAL AND OPTICAL CHARACTERIZATION OF Ni/NiO NANOCHAINS

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In recent years, among transition metal oxides nickel oxide (NiO) nanostructures have attracted much attention owing to its unique optical, electrical, catalytic and magnetic properties. It is a promising candidate for wide range applications like gas sensors, supercapacitor, anode material for Li-ion batteries, catalyst, dye sensitized photocathodes, optoelectronic devices, etc. [1, 2].

In the present work, Ni / NiO nanochains were synthesized under external magnetic field. The magnetic field intensity was about 25 mT. Initially, Ni nanochains were prepared by chemical reduction method utilizing sodium borohydride and hydrazine hydrate as reducing agents and then thermal oxidized at different temperatures (400, 500 and 600 °C) for 2 h. XRD was used to determine phase structure and composition of samples. In the XRD pattern of Ni nanochains, three diffraction peaks were observed at 44, 52 and 76 ° due to the cubic structure of Ni. The large peak width is due to the small particle size. The particle size calculated from XRD is 5.82 nm.

After thermal annealing at 400 °C, in the diffractogram of sample nickel-related peak intensity has increased and the width of the peak is reduced. It is attributed to the increase in particle size at high temperature. The crystallite size was calculated as 18.4 nm for the peak at 44 °. Additionally, the small intensity peaks of nickel oxide was observed at 37, 43 and 62 ° corresponding to (111), (200) and (220) planes. When the temperature was raised to 600 °C, the intensity of the nickel oxide peaks increased and considering the peak at 43°, particle size has been estimated as 15.3 nm. UV-Vis spectroscopy analysis was carried out in order to determine optical band gap energy of samples. The optical band gaps of Ni / NiO nanochains annealed 400, 500 and 600 °C temperature are 3.87 eV, 4.1 and 3.90 eV, respectively. SEM analysis was employed to investigate the morphology of the samples. From SEM measurements chain-like morphology was observed and the chain has a necklace-like shape assembled by nickel particles.

Before thermal annealing, the diameter of Ni nanochains is in the range of 56.1 – 88.6 nm and the length is about 6.92 µm. After thermal annealing at 400 °C, the diameter of Ni / NiO nanochains increased up to 103 nm. It is obvious that application of external magnetic field has significant influence on the formation of nanoparticles as chain-like structure. So that the magnetic moment of each particle is aligned in the direction of the external field and chain-like structure was formed.

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CARBON NANOTUBES AND GRAPHENE HYBRID MATERIALS SYSTEMS FOR MULTIFUNCTIONAL APPLICATIONS IN ENERGY AND ENVIRONMENT

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Currently we face considerable global challenges in energy and environment compatibility and sustainability [1]. In order to answer some of these challenges there is an urgent need to use less energy and to activate energy sources with lower GHG intensity. Carbon nanotubes and graphene are almost perfect molecules with truly amazing combinations of thermal, electrical and structural properties [2 – 4]. In order to achieve their full potential, they need to be fully integrated hybrid materials in all sorts of matrices.

Full integration requires their development beyond conventional composites so that the level of the non-nanomaterial is designed to integrate fully with the additions of nanotubes and graphene. Here the nanomaterials are part of the matrix rather than a differing component, as in the case of conventional composites.

In order to advance the development of multifunctional materials and to integrate nanotubes and graphene, this research is focused on the simultaneous control of the nano-architecture, structural properties, thermal and electrical conductivity of fully integrated hybrid materials. These hybrid material systems are designed to surpass the limits of the rules of mixtures in conventional composite design.

The goals are to implement multifunctional 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 fluids, nanolubricants, structural applications of polymeric and ceramic matrices.

Applications in energy systems and subsystems such as transportation, wind, solar and subsystems such as capacitors and batteries as well as other material systems are presented and discussed.

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**PLASMA-ASSISTED PREPARATION OF NANO-ZrC@C
COMPOSITES FROM Zr-LOADED SULPHONATED
STYRENE-DIVINYLBENZENE CO-POLYMERS**

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A convenient method has been developed to prepare nano-ZrC / C composites with adjustable ZrC / C ratio based on a plasma-assisted heat-treatment of zirconium-loaded styrene-divinylbenzene (STY-DVB) copolymers with various DVB content. The first step of preparation is a heat treatment in a tube furnace 1000 and 1400 °C for 2 h to prepare nano-ZrO₂ / C composites with 30 – 60 nm ZrO₂ particle size.

Subsequent plasma-assisted heat-treatment of nano-ZrO₂ / C mixtures prepared in a tubular furnace under N₂ at 1000 °C for 2 h from the 8 % DVB containing and fully Zr-loaded resin in He or H₂ atmosphere resulted in nano-ZrC_{0.93} / C composites with 10.5 (RF-He) (C / Zr = 73) or 12.9 % (RF-H₂) (C / Zr = 58) ZrC_{0.93} content.

Keeping DVB content, degree, Zr-loading and the thermal treatment conditions which have influence on the and properties of nano-ZrO₂ / C intermediates, a reproducible and easy route is given to prepare / C products with ~ 20 nm size. The role of degree of sulphonation, the positions of sulphonated groups, the DVB content, and the Zr-loading in the loading and chemical speciation of zirconium bound on the polymer are also discussed.

EFFECT OF FULLERENE 60 ON ELECTRICAL, MECHANICAL AND WEAR CHARACTERISTICS OF EPOXY COMPOSITE

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Effect of weight fraction (WF, mg/dL) of fullerene 60 (C_{60}) on electrical, mechanical and wear characteristics of epoxy nanocomposites (ENCs) was investigated.

For this purpose, a series of ENCs was prepared through dispersion of various WF of C_{60} into epoxy resin in presence of toluene co-solvent. This was followed by curing of C_{60} / epoxy composition with polyamine. Dispersion of C_{60} into epoxy matrix and onward formation of ENCs and was revealed through atomic force microscopy. ENCs have rendered a rising trend in DC conductance ranging 98.32 to 0.79 $\mu\text{S}/\text{cm}$ with electrical percolation threshold at 200 WF of C_{60} (**Figure 1**). Their compressive, impact, tensile, and strength, were enhanced and at 200 WF of C_{60} .

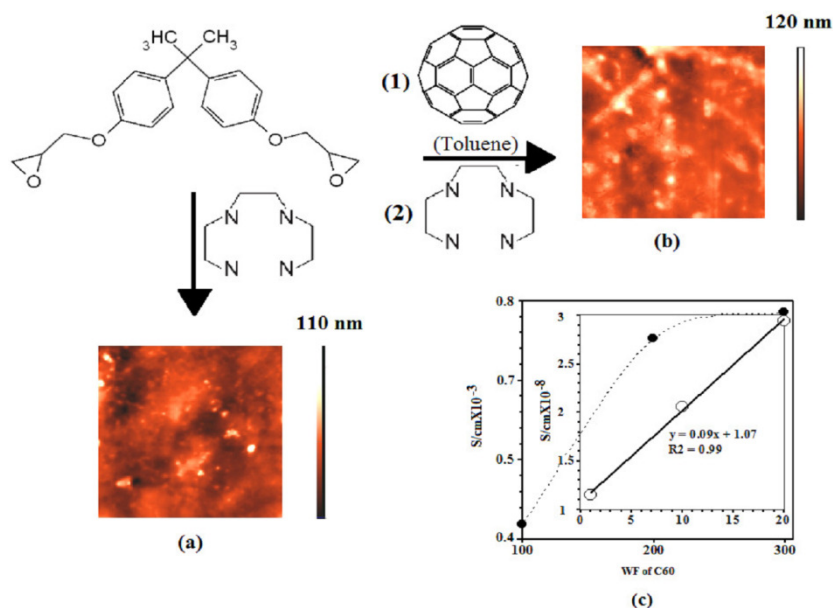


Figure 1. AFM of cured epoxy (a), ENCs with 200 WF of C_{60} (b) and effect EF of C_{60} on DC.

In general, ENCs are shown a marginal modification in their compressive strength by 3.30 % over cured epoxy (CE). However, their impact and tensile strengths were largely improved to 28.75 and 53.25 % over CE. The study provides a novel method of modification in electrical and mechanical behavior of epoxy through introducing C_{60} .

BIOSYNTHESIS OF SILVER NANOPARTICLES USING EXTRACTS OF “HAIRY” ROOTS OF MEDICINAL PLANTS

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Synthesis of nanosized materials especially silver nanoparticles for their different applications are now of great interest. The synthesis of nanoparticles using biological agents is becoming more attractive as an alternative to traditional synthetic methods. Biosynthesis of nanoparticles involves using an eco-friendly, green-chemistry-based approach that makes use of bacteria, fungi, etc. The genetic transformation using wild-type *Agrobacterium rhizogenes* allows obtaining hormone-independent root cultures after the transfer the *roll* genes to the plant genome. These genes are the inducers of secondary metabolism. Thus, the resulting “hairy” roots can synthesize various compounds, in particular flavonoids, in quantities that are several times higher than their concentration in the mother plants, and have significantly greater biological (including reducing) activity. So, these roots are the donors of the compounds with a strong reducing activity and can be included in the biotechnology of NPs especially silver-based.

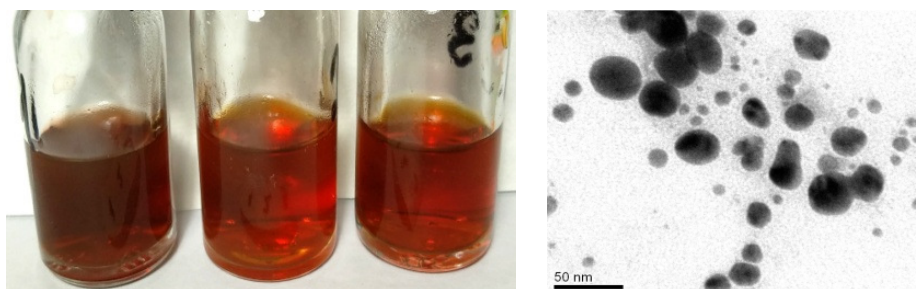


Figure 1. Obtained AgNPs using *Artemisia* “hairy” root extracts.

In this work the “hairy” root extracts of *Artemisia* spp were used for synthesis of silver nanoparticles (AgNPs). The AgNPs produced were further characterized using UV, FTIR, and TEM methods. TEM analyses confirm the synthesis of AgNPs which have spherical shape and an average size of presumably 10 – 50 nm (**Figure 1**). In addition, the final AgNPs including the average diameter, dispersion and optical properties can be easily controlled by changing the main parameters in the process. Total flavonoid content in *A. tiliifolia* “hairy” root lines was up to 58.87 ± 9.30 mg RE/g DW and 32.05 ± 3.80 mg RE/g DW in the control roots. The reducing properties of the extracts were found to correlate with total flavonoid content. Therefore, the extracts of “hairy” root cultures of *Artemisia* spp. can produce compounds with high reducing activity are an excellent candidate for “green” synthesis of various nanoparticles.

COUPLED VERTICAL CYLINDRICAL QDS WITH DOUBLE MODIFIED PÖSCHL–TELLER POTENTIAL IN AXIAL ELECTRIC FIELD

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Consider the motion of electron in a coupled vertical cylindrical QDs, with double modified Pöschl–Teller potential (MPTP) (**Figure 1**) in axial electric field [1, 2].

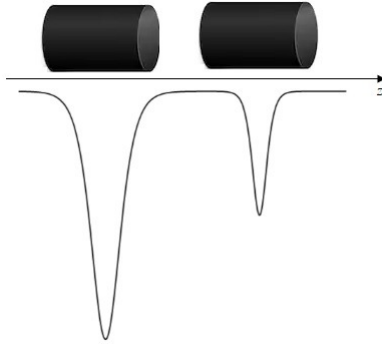
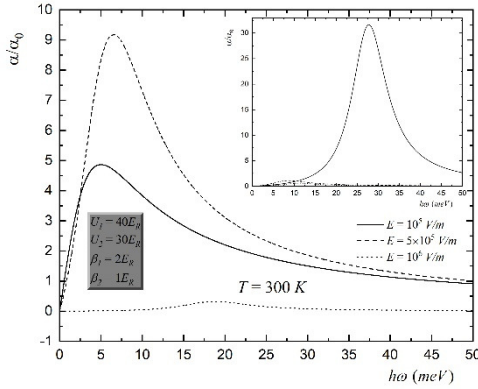
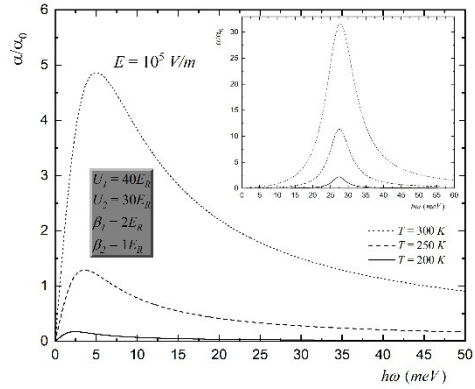


Figure 1. Coupled vertical cylindrical QDs with double MPTP.



(a)



(b)

Figure 2. Dependence of absorption coefficient on frequency for the light (inserts: heavy) hole to electron transitions) for different electric fields **(a)** and temperatures **(b)**.

We also investigated some optical parameters of this system (absorption and PL coefficients) – see **Figure 2**. $U_{1,2}$ and $\beta_{1,2}$ are depths and half-widths of the first and second MPTP, respectively.

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INFLUENCE OF TEMPERATURE IN THE GROWTH PROCESS OF $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ / PVA NANOCOMPOSITES THROUGH SILAR METHOD

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II–VI semiconductor materials have been great interest due to unique properties and large application fields. These groups' materials have wide band gap energy and used high-performance optoelectronics and optics devices. Light emitting diodes, laser diodes, solar cell, sensors, high power electronic devices, electronics devices, SAW oscillator and etc. are application field of these materials [1]. $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ ternary nanomaterials are shown properties in the between CdS and ZnS binary nanomaterials. Ternary $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanomaterials exhibit improved structural and optical properties and are used potentially useful as a window layer in solar cells, photoconductive devices [2]. In this study, to determine the influence of reaction temperature, CdZnS nanomaterials were synthesized by SILAR method at different growth temperature.

Polyvinyl alcohol (PVA) was taken as initial sample. The cation sources were selected cadmium acetate dihydrate $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ and zinc acetate dihydrate $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$, sodium sulfide Na_2S as anion source and ethylene glycol was used as washing agent and solvent. The sorption duration was chosen 40 min. For all processes in the experiments, the cycle was selected as 5 periods. The reaction were carried out for different ratios depending of x value in $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ nanomaterials at room temperature, too. For to determine of influence of temperature on the properties of $\text{Cd}_{0.2}\text{Zn}_{0.8}\text{S}$ / PVA nanocomposites were synthesized at temperatures 25, 40 and 65 °C.

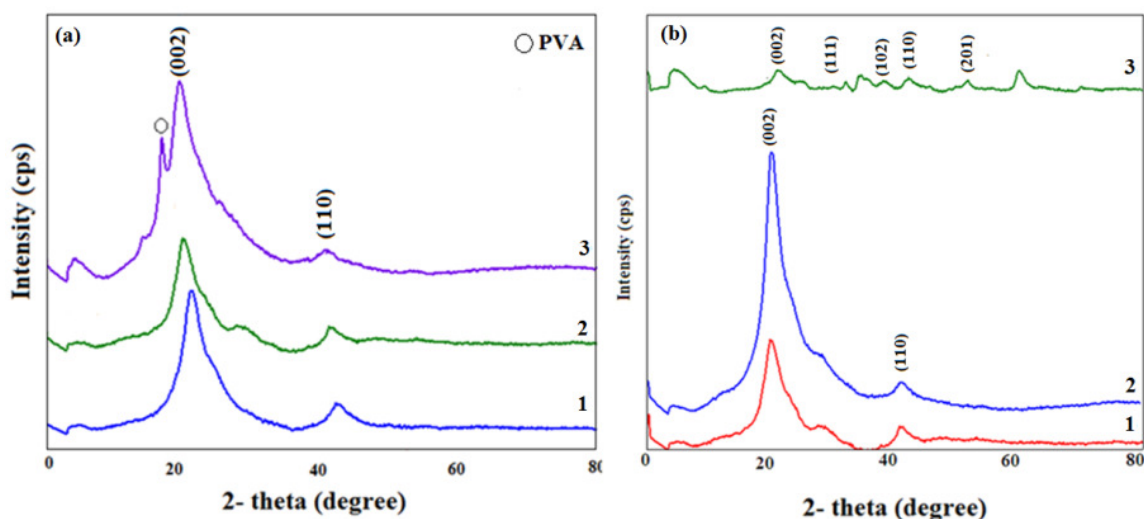


Figure 1. XRD pattern of (a): $\text{Cd}_x\text{Zn}_{1-x}\text{S}$ / PVA for x – (1) 0.1, (2) 0.2, (3) 0.8 and (b): $\text{Cd}_{0.2}\text{Zn}_{0.8}\text{S}$ / PVA – for T – (1) 25, (2) 40, (3) 65 °C.

In **Figure 1a**, the observed peaks are belong to wurtzite structure (JCPDS card no: 40-0835) and confirms the formation of CdZnS crystal, and respectively indexed with (002) and (110). The sample which synthesized at 40 °C temperature (**Figure 1b-2**) preserved its structure and compatible to wurtzite structure of $\text{Cd}_x\text{Zn}_{1-x}\text{S}$. But at 65 °C temperature (**Figure 1b-3**), the new peaks were formed which belong to wurtzite structure of $\text{Cd}_x\text{Zn}_{1-x}\text{S}$. The results show that, at high temperatures, the formation process of ternary nanocomposites is good.

Table 1. Average sizes and band gap values of samples.

Samples	Average size D from XRD, nm	Band gap values E_g , eV
$\text{Cd}_{0.1}\text{Zn}_{0.9}\text{S} / \text{PVA}$	3.2	3.15
$\text{Cd}_{0.2}\text{Zn}_{0.8}\text{S} / \text{PVA}$	3.3	3.05
$\text{Cd}_{0.8}\text{Zn}_{0.2}\text{S} / \text{PVA}$	3.4	2.8
$\text{Cd}_{0.2}\text{Zn}_{0.8}\text{S} / \text{PVA}$ $T = 40\text{ }^\circ\text{C}$	4.3	3.14
$\text{Cd}_{0.2}\text{Zn}_{0.8}\text{S} / \text{PVA}$ $T = 65\text{ }^\circ\text{C}$	2.6	2.37

The band gap values of the obtained samples are decreases with increasing of particle size (**Table 1**). From XRD results observed that, at high temperature, the growth process is good than selected different growth temperature. With increases of x value, the values of the band gap are diminished.

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SILVER–SILVER SULPHIDE HYBRID NANOWIRES: FABRICATION, STRUCTURE AND PHYSICAL PROPERTIES

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Hybridization of semiconductors and noble metals is an attracting research topic because it leads to synergistic effects to enhance performance of materials. Hybridization of silver modulates the structure of the bandgap of silver sulphide at the interface and makes separation and transfer of charges easy and suppresses recombination of the charge carriers because electrons which are excited to the conduction band of silver sulphide easily transfer into silver at the boundary of silver-silver sulphide and hold position there until being utilized [1].

In this study, a facile fabrication of silver-silver sulphide hybrid nanowires is presented. As prepared silver nanowires by the polyol method is simply mixed with sulphur ions containing solution. Hybrid nanowires are investigated by SEM, EDX, XRD and UV-Vis to confirm successful fabrication and to analyse the physical properties.

Inorganic semiconductors are brittle thus hard to be used for flexible or stretchable conditions. But as reported, silver sulphide shows much ductility [2]. This ductile property of silver sulphide may also contribute to fabrication of mechanically robust flexible devices.

Silver nanowires are synthesized by according to the polyol method of a literature [3] with some modifications. Ag–Ag₂S hybrid nanowires are successfully fabricated by a simple mixing process between Na₂S aqueous solution and AgNWs which are prepared by the polyol method. Ethanol which is good solvent for PVP facilitates sulphur ions to approach the surface of AgNWs because it stretches out to provide room for approaching. Morphologies of Ag–Ag₂S hybrid nanowires are investigated by SEM which reveals Ag–Ag₂S hybrid nanowires have larger diameter than that of pristine AgNWs, which means uniform coverage of Ag₂S but show rough surface which is ascribed to Ag₂S grown by Oswald ripening. UV-Vis absorbance peaks are red-shifted and the absorbance graphs are broadened as hybridization proceeds because of formation Ag₂S on the surface of AgNWs. This phenomenon results from change of dielectric constant of Ag₂S nanocrystals which grow on AgNWs as the hybridization proceeds and from change of band gap energy of Ag₂S according to its size at the nano-size regime. This fact makes Ag–Ag₂S be a better photocatalyst because it can be active under a broad range of light and also the range of absorbance of light can be adjustable by concentration and time of reaction. XRD data show peaks which belong to Ag₂S crystals and lose peaks which belong to AgNWs as hybridization proceeds.

A promising photocatalyst, Ag–Ag₂S hybrid nanowires will be further studied to photocatalytic applications for generating energy and cleaning environment. Plasmon oscillation on Ag nanoparticles in different environments were considered. It has been shown that the frequency of oscillation depends on the polarity of the environment. This is also due to the effect of the dipole electron interaction between the the environment and free electrons in nanowire.

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BEYOND THE DIRAC CONES: ZERO EFFECTIVE MASS CARRIERS IN 2D MATERIALS WITH HYPERBOLOID CONDUCTION BANDS

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The emergence of Dirac cones in graphene is one of the most striking examples when physics and geometry are inevitably and profoundly intertwined in the landscape of the energy bands of two-dimensional (2D) materials. In the vicinity of those cones the energy-momentum dispersion relation becomes linear which gives rise to exotic and potentially useful new phenomena.

Here we examine the potential of the hyperboloidal band structure of a 2D crystal lattice for emulating massless Dirac carriers. Though counterintuitive, when in momentum space the band energy is shaped as a hyperboloid of one sheet, the linear dispersion relation holds again. Moreover, now it can provide with new unprecedented avenues for guiding and localization of massless charge carriers in the conduction band.

The possibilities of band structure engineering to realize the corresponding energy landscape in diverse 2D materials, their heterostructures, metasurfaces and metamaterials are discussed.

ECO-SAFE FORMULATIONS BASED ON CHITOSAN AND HYDROXYCINNAMIC ACIDS FOR SEED TREATMENT

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Modern technologies for growing vegetable crops involve the replacement of chemical plant protection products by biologically active compounds that have properties of growth regulators and plant resistance inducers. They stimulate growth, development and productivity of crops, induce plant resistance to abiotic and biotic stresses, and improve product quality. The eco-friendly formulations based on polysaccharides and hydroxycinnamic acids are promising for sustainable agriculture applications [1].

The aim of this work was to study the effect of seed treatment with hydroxycinnamic acids (0.1 – 100 µM ferulic or caffeic acid), chitosan (30, 250 and 1200 kDa) and their formulations (mixtures and conjugates) on the initial growth of cucumber seedlings (*Cucumis sativus* L.). The chitosan–ferulic acid (Chit–FA) and chitosan–caffeic acid (Chit–CA) conjugates with different coupling ratio (from 0.5 to 5.0 %) were synthesized by standard EDC-crosslinking protocol [2].

It was shown, that the ferulic and caffeic acids at a concentration of 10 µM, chitosan with a molecular weight of 30 kDa, as well as their mechanical mixtures exhibit a positive effect on the growth parameters of seedlings. Thus, coating of cucumber seeds with the mixture of chitosan and 10 µM ferulic acid increased the root mass and length by 14 and 12 % respectively, shoot length by 7 % compared to control plants. The coating of cucumber seeds with combinations of chitosan and 10 µM caffeic acid increased the root mass by 9%, weight and shoot length by 10% compared to control plants. For Chit–FA and Chit–CA the greatest stimulating effect was observed for coating seeds with conjugates containing 4.0 – 5.0 % of FA or CA. It was found that the Chit–FA and Chit–CA conjugates had the same effect on morphometric parameters of cucumber seedlings as a mixture of chitosan and hydroxycinnamic acids. Individual hydroxycinnamic acids reduced the activity of proteolytic enzymes in leaves while the activity of their inhibitor increased. Whereas the use of hydroxycinnamic acids and 30 kDa chitosan mixtures led to an increase in the activity of proteases compared to pure chitosan, and a mixture of ferulic acid and chitosan caused an enhance in the activity of proteases compared to control. The activity of the protease inhibitors in plant leaves after treatment seeds with pure chitosan or mixtures of chitosan and hydroxycinnamic acids remained almost constant.

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PYRAMIDS AND COOTIE CATCHERS: NEW MASSLESS FERMIONS IN 2D MATERIALS

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Dirac-like electronic states are the main engines powering the tremendous advances in research of graphene, topological insulators and other materials with these states. Zero effective mass, high carrier mobility and numerous applications are some consequences of linear dispersion that distinguishes Dirac states.

Here we report a new class of linear electronic bands in two-dimensional materials with zero effective mass and sharp band edges never seen in solid state matter before, and predict stable materials with such electronic structure utilizing symmetry group analysis and *ab initio* approach [1]. We make a full classification of completely linear bands in two-dimensional materials and find that only two classes exist: Dirac fermions on one hand and pyramidal-like and cootie catcher-like states on the other hand.

The new class supports zero effective mass and hence high carrier mobility similar to that of graphene, anisotropic electronic properties like that of phosphorene, and robustness of states with respect to electronic correlations.

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**EFFECT OF COLLOIDAL METAL NANOPARTICLES
ON BIOSYNTHETIC ACTIVITY OF LIQUID-CULTURED
Inonotus obliquus (ACH.: PERS.) PILAT**

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Currently, various nanomaterials are being actively studied; in particular, colloidal solutions of biologically active metals have been obtained using nanotechnologies, which exhibit anti-stress properties and increase the resistance of animal, plant, bacterial, and micromycete cells to various adverse factors.

However, there is still no information on the possibility of the use of nanomaterials in macromycetes cultivation biotechnology. Therefore, studying the possibility of increasing the efficiency of the synthesis of biologically active substances by medicinal mushrooms by using metal nanopreparations, which, unlike their salts, are potentially less toxic, should be of relevance. In our work, we studied the effect of colloidal solutions of Ag (AgNPs), Fe (FeNPs), and Mg (MgNPs) nanoparticles on the growth and biosynthetic activity of the medicinal macromycete *Inonotus obliquus*, which is a source of antioxidant, hepato-, chemo-, and radioprotective and antitumor components.

The addition of all investigated metal nanoparticles to the culture medium significantly stimulated the growth activity of medicinal mushroom *I. obliquus*. Biomass value increased up to 46 – 69 % compared with the control (without NP addition to the medium). However, it was found that the level of the accumulation of biologically active compounds depended on the metal used in the experiment. FeNPs and MgNPs increased the number of endopolysaccharides by 62 and 46 %, respectively, but reduced the exopolysaccharides elevenfold. AgNPs inhibited the synthesis of both exo- and endopolysaccharides (by 5.6 times and 23 %, respectively). The presence of AgNPs and FeNPs in the medium resulted in the reduction of flavonoid content in the mycelium twofold and by 27 %, respectively.

Conversely, MgNPs stimulated flavonoid synthesis in mycelia up to 35.9 %. All nanoparticles stimulated the synthesis of melanin pigments in *I. obliquus* (FeNPs – 25, MgNPs – 80, and AgNPs – 140 %). The data obtained in the experiments justify the effect of metal NPs as growth regulators and activators of biosynthetic activity of *I. obliquus*. These data can be used for the establishment of environmentally friendly and effective biotechnology of *I. obliquus* macromycete in vitro cultivation to produce compounds with medicinal properties.

INGaAs ALLOYS FOR USE IN THERMOELECTRICITY

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The development of new spheres of semiconductor technology, especially, nanotechnology, needs the materials with intermediate properties of binary III–V compounds. Among them InGaAs alloys are practically applied the basic active component for manufacture nanotech products, in particularly, thermoelectricity. Developing thermo electrical batteries has become a major research topic due to their broad applications as heat pumps and power generators. The particular attention to InGaAs alloys are defined for their basic thermoelectric transport parameters. These are the electrical and thermal conductivities and the Seebeck coefficient.

Semiconductors do not, in general, exhibit uniformly good thermoelectric properties over the large temperature ranges necessary for high power efficiencies [1, 2]. Therefore much attention has been directed towards materials, such InGaAs alloys, which are thermoelectrical effective over relatively narrow temperature ranges. Combining such low temperature materials with high temperature ones in the construction of thermocouples branches in a sandwich arrangement let obtain optimum thermoelectric performance.

Driven by emerging demands for thermobatteries research has been conducted on InGaAs alloys. Homogeneous InGaAs alloys were produced by direct fusion process of InAs and GaAs components and using the crystal growth method [3]. Physical measurements of the electrical and thermal conductivities and the Seebeck coefficient have been implemented. It has been obtained the Seebeck coefficient and electric resistivity is higher in the ternary than in the binary InAs; this is advantageous for the design of thermoelectric devices.

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**PECULIARITIES OF THE BINDING OF CATIONIC
meso-SUBSTITUTED PORPHYRINS TO POLY(P)
AND SYNTHETIC POLYNUCLEOTIDES**

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Water-soluble tetracationic *meso*-porphyrin, TMPyP⁴⁺, and its tricationic derivative, TMPyP³⁺, are macrocyclic compounds with high biological activity and unique photophysical properties which effectively bind to nucleic acids (NA) stabilizing and changing their local structure. Three binding modes were defined for interaction of the porphyrin with NA, namely (i) intercalation of the dye between nucleic bases, (ii) its incorporation into the helix groove and (iii) outside electrostatic binding of the dye to NA phosphate backbone with / without self-stacking.

The manner in which the porphyrin binds to NA is known to depend on the structure of its substituents, the presence and the type of metal ion at the center of porphyrin core, NA type, ionic strength of the solution, as well as on phosphate-to-dye ratio. The presence of planar macrocyclic core in the porphyrin structure determines an ability to form non-covalent self-organized multimolecular π -stacked assemblies on the surface of NA with strong interaction between neighboring molecules, which play a significant role in charge and exciton transfer and can act as artificial light-harvesting devices.

The peculiarities of binding of TMPyP⁴⁺ and TMPyP³⁺ porphyrins to single-stranded inorganic polyphosphate, poly(P), as well as to synthetic polynucleotides including single-stranded poly(A), double-stranded poly(A)·poly(U) and poly(G)·poly(C), four-stranded poly(G) were studied using experimental methods of absorption spectroscopy, polarized fluorescence, steady-state light scattering and resonance Raman spectroscopy as well as molecular modeling (DFT calculations).

COMPOSITE BUBBLE STRUCTURES BASED ON BORON NITRIDE AND OTHER COMPOUNDS FORMED UNDER CONCENTRATED LIGHT IN FLOW OF NITROGEN FROM BORON AND INACTIVE METAL POWDERS

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A Continued miniaturization of electronic devices and increased power density have stipulated the increased demands for operational lifetime and reliability of electronic systems. These trends motivate researchers to work on different aspects of the group-III nitride semiconductors such as boron nitride (BN).

BN exhibits unique electronic properties such as a low dielectric constant, high thermal conductivity, and chemical inertness. Unfortunately, BN nanostructures have not been widely studied since the major application areas of BN are considered to be in thermal management, graphene electronics, and mechanical applications. Nevertheless that the indirect bandgap of BN in the UV with the possibility of its tuning via stoichiometry, defects and doping suggests its rich application.

There are some features in the formation of compounds of boron with different metals. Boron does not form continuous solid solutions with any metal. It weakly interacts with copper and completely does not interact with aurum, argentum, zinc subgroup metals, indium, thallium, tin, lead and bismuth. Boron forms a eutectic mixture with metallic gallium and gives borides, which formed in accordance with the rules of valency only with active metals.

It was found formation composite bubble structures based on boron compounds under concentrated light in flow of nitrogen from boron and inactive metal powders. These structures can exhibit very high surface area, large pore volume, and excellent chemical stability. Research on synthesis, structures and properties of various composite bubble structures has shown that they are promising materials for many applications, such as energy storage, gas storage, heterogeneous catalysis and sensing. Their potential applications in energy-related devices and processes will bring innovation in development of supercapacitors, lithium ion batteries, electrocatalysts, photocatalyst, gas sensing, water treatment, solar cells, and carbon dioxide capture.

Therefore, synthesis of new composite bubble structures based on B compounds and inactive metals under concentrated light in nitrogen flow can be considered as an outlook direction of development in terms of future challenges and potential prospects towards industrial applications.

**DIELECTRIC PROPERTIES OF CERAMICS ON THE
BASIS OF PEROVSKITES OF TYPE $A(R_{0.5}B_{0.5})O_3$
(A: Ba^{2+} , Sr^{2+} , Ca^{2+} ; R: Nd^{3+} , Sm^{3+} , B: Nb^{5+} , Ta^{5+})**

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The general requirements for ceramic materials used in microwave technology are as follows: a wide range of dielectric permittivity (ϵ) values with near to zero temperature coefficient of this parameter ($TC\epsilon$) as well as the small dielectric losses, leading to high values of quality factor ($Q \sim 1 / tg\delta$). It is known that the complex perovskites of the $A(B'_nB''_m)O_3$ type can provide required properties and other dielectric parameters appropriate for applications in the microwave range. This work presents the results of investigations of microwave properties of the samples of ceramic materials based on solid solutions of the $A(R_{0.5}B_{0.5})O_3$ composition (A = Ba^{2+} , Sr^{2+} , Ca^{2+} ; R = Nd^{3+} , Sm^{3+} ; B = Nb^{5+} , Ta^{5+}) and prepared by the two-stage ceramic technology [1].

The study of the morphology of the samples has shown that the average grain size increases as the ionic radius of cation in the A sublattice increases and varies in the range 2 – 5 μm . It was found that the larger the grain size of ceramics of a certain composition is, the higher the values of dielectric permittivity are. Temperature studies of dielectric permittivity ϵ in the interval from – 30 °C to + 300 °C have shown the high temperature stability of this value for all samples studied. In particular, for Sr-based ceramics $Sr(Sm_{0.5}Ta_{0.5})O_3$ the $TC\epsilon$ value in this temperature range is practically equal to zero. The presence of Sm^{3+} ions in the B-sublattice leads to monotonically increasing character of the temperature dependence of dielectric loss tangent ($tg\delta$), which is less pronounced for compositions with Barium or Calcium in A position.

As a result of investigations, a number of new ceramic dielectric materials is prepared on the basis of compositions $A(R_{0.5}B_{0.5})O_3$ with perovskite structure. These materials possess very low values of dielectric loss tangent $tg\delta$ and high thermal stability of dielectric permittivity ϵ in the wide range of temperatures. Such peculiarities make them perspective from the point of view of practical use in the microwave devices of various purposes and applications.

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DEVELOPMENT OF COMPOSITIONS OF GEOPOLYMER BINDERS BASED ON ROCKS OF GEORGIA

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Global growth in OPC production is inevitably accompanied by an increase in the negative anthropogenic impact on the planet's ecology and irrational consumption of energy carriers. One of the ways to solve these problems is the use of geopolymers – alkali-activated aluminosilicate binders based on local non-scarce rocks and granular slags of the metallurgical industry.

The purpose of this work is to study the clay rocks of Georgia for the synthesis of geopolymer binders. For the study were used clay rocks widespread in Georgia: shale, argillite and fusible clay [1 – 5]. **Table 1** shows the chemical compositions of the studied materials: No. 1 – Shale, No. 2 – Argillite, and No. 3 – Clay.

Table 1. Chemical composition of clay rocks, mas. %.

No.	LOI	SiO ₂	TiO ₂	Al ₂ O ₃	Fe ₂ O ₃	FeO	Mn ₂ O ₃	CaO	MgO	SO ₃	Na ₂ O	K ₂ O
1	4.50	59.95	0.89	17.30	3.45	3.65	0.59	1.53	2.43	0.30	2.20	2.20
2	7.01	47.19	–	15.90	13.36	–	0.10	6.30	4.10	1.39	2.86	1.30
3	10.60	52.84	–	15.07	6.47	–	–	7.06	2.49	1.36	1.19	2.17

As a result of the studies, a heat treatment regime for clay rocks was developed and various compositions of geopolymer binding materials were obtained on their basis. It was found that heat treatment of the geopolymer binders significantly increases the mechanical strength of the latter.

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MODIFICATION OF CLAY ROCKS FOR OBTAINING A HIGHLY ACTIVE POZZOLANIC ADMIXTURE

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Cement production is associated with high fuel and energy resources and the use of mineral (pozzolanic) admixtures in Portland cement is one of the most effective solutions to these problems. Due to the limited distribution of natural pozzolans in Georgia, it is of practical interest to use local raw materials and to develop ways to increase its pozzolanic activity.

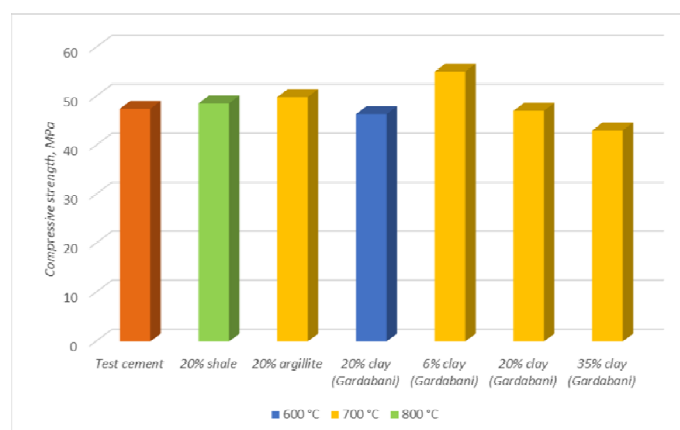


Figure 1. Hydraulic activity of cement samples after 28 days hardening.

Modes of thermal modification of clay rocks (ordinary fusible clays, argillites and shales) have been developed, after which, they can be used as a pozzolanic admixture in Portland cement [1 – 5]. The use of these admixtures to 35 % will make it possible to reduce the share of clinker in Portland cement without reducing the mechanical strength, and with the addition of about 6% of modified clay rocks, a significant increase in the mechanical strength of cement is observed (**Figure 1**).

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SYNTHESIS OF BiFeO_3 FERROELECTRIC FROM $\text{Bi}_{25}\text{FeO}_{39}$ PRECURSOR AND Fe_2O_3 OXIDE

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Bismuth ferrite BiFeO_3 is one of the most known multiferroic and it exhibits the ferromagnetic and at the same time ferroelectrical properties. That's why it can be used for synthesis of new magnetoelectric materials with high values of electrical polarization and magnetization at room temperature. Despite of constant investigating BiFeO_3 synthesis methods and its properties obtaining of single phase bismuth ferrite BiFeO_3 is a difficult task because it always contains impurity phases of $\text{Bi}_2\text{Fe}_4\text{O}_9$ and $\text{Bi}_{25}\text{FeO}_{39}$ [1].

We have developed the solid-state reactions method of synthesis of BiFeO_3 multiferroic from $\text{Bi}_{25}\text{FeO}_{39}$ precursor and Fe_2O_3 oxide and investigated influence of various modes of heat treatment on crystal structure of BiFeO_3 and the optimum conditions of synthesis are chosen. The method includes the next stages. First the $\text{Bi}_{25}\text{FeO}_{39}$ precursor was synthesized by solid-state reaction at 750°C for 4 h in air from the corresponding iron and bismuth oxides. By X-ray powder diffraction analysis it was determined, that obtaining $\text{Bi}_{25}\text{FeO}_{39}$ had a single phase and cubic crystal structure of sillenite. Then the bismuth ferrite BiFeO_3 was synthesized at the same conditions: by solid-state reaction at 750°C for 4 h from obtained $\text{Bi}_{25}\text{FeO}_{39}$ and Fe_2O_3 oxide. This stage included compulsory grinding of $\text{Bi}_{25}\text{FeO}_{39}$ with ethanol and mixing it with Fe_2O_3 oxide powder in required proportions. This mixture was pressed in tablets, and only then heat treatment applied.

It was found that the synthesized BiFeO_3 sample had a crystal structure of rhombohedral perovskite and unfortunately it was not single phase. Because BiFeO_3 samples had a little quantity of impurity phases $\text{Bi}_2\text{Fe}_4\text{O}_9$ and $\text{Bi}_{25}\text{FeO}_{39}$ additional high temperature treatment with various modes carried out. It has been established that additional heat treatment at 800°C for 2 h led to decrease quantity impurity phases from 5 to 2 – 3 %.

So, the developed ceramic or solid-state reaction method of synthesis of BiFeO_3 multiferroic from $\text{Bi}_{25}\text{FeO}_{39}$ precursor and Fe_2O_3 oxide allows to reduce time and synthesis temperature in comparison with ceramic method of BiFeO_3 synthesis from Bi_2O_3 and Fe_2O_3 oxides, and also allows to reduce the quantity of impurity phases.

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OPTICAL PROPERTIES OF POLYVINYL ALCOHOL FILMS MODIFIED WITH A Fe₃O₄–GOLD COMPOSITE

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The effect of the Fe₃O₄–Au composite on the optical properties of stained with dichroic dyes Chicago Sky Blue (GSB), (6-amino-4-hydroxy-3-[[4-(phenyl)azo]phenyl]-2-naphthalene sulfonic acid) (M_{3h}) and (monosodium mono (4-(2-(2-(2-chloro-1-(2-(1-(4-sulfonate-butyl))-3,4-dihydroquinolin-2(1H)-ilidene)ethylidene)-1H-inden-3-yl)vinyl)-3,4-dihydro-quinolin-1(2H)-yl)butane-1-sulfonate) (IR-3) polyvinyl alcohol (PVA) films was investigated.

The Fe₃O₄–Au composite, in the form of iron oxide nanorods surrounded by gold nanoparticles, was synthesized according to the procedure [1]. Colored anisotropic PVA films modified with Fe₃O₄–Au were obtained similarly [2], and their polarizing efficiency (PE) [2] was calculated at a wavelength λ , nm (Table 1).

Table 1. Polarizing ability of colored PVA films modified with Fe₃O₄–Au composite.

Dye/(Fe ₃ O ₄ –Au)	C, mas.% / V, ml	λ , nm	PE, %
CSB	0.3	594 – 690	90 – 97
M _{3h}	0.2	300 – 610	90 – 99
IR-3	0.2	781 – 785	94
CSB/(Fe ₃ O ₄ –Au)	0.3 / 4.5	545 – 704	90 – 99
M _{3h} +CSB+IR-3/(Fe ₃ O ₄ –Au)	Σ 0.3 / 1.5	400 – 827	90 – 97

The inclusion of Fe₃O₄–Au in the Chicago Sky Blue PVA-stained matrix leads to a shift in the wavelength of the films in the near IR region of the spectrum (up to 704 nm) and an expansion of the spectral range in the visible region of the spectrum (up to 545 nm) compared to the GSB sample (594 – 690 nm) (Table 1). A PVA film of a mixture of three dyes and Fe₃O₄–Au polarizes light (PE = 90 – 99 %) in a rather wide spectral range of 400 – 827 nm (Table 1). The UV-light photostability of colored films in the presence of magnetite nanoparticles [2] determines their suitability for various optical applications.

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THE CATALYTIC ACTIVITY OF THE MAGNETIC Fe_3O_4 / CeO_2 COMPOSITE IN THE REACTION [3 + 3] CYCLOCONDENSATION

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Due to the large specific surface area, nanocatalysts have high activity and selectivity, as well as a long term of use [1]. Also, by adding a magnetic component to a composite containing cerium dioxide, it is possible to cyclically use such a catalyst.

The study is devoted to develop a method of design of composite nanocatalyst based on magnetite and cerium dioxide Fe_3O_4 / CeO_2 – to obtain derivatives of 2-amino-pyrimidine – organic compounds whose high antitumor activity potential causes constant interest in developing rational methods for their preparation. The composite was synthesized using a one-stage ultrasonic synthesis method [2]. The composite was characterized by SEM, XRD, and VSM methods. The studies showed the composite consists of agglomerates of nanosized particles of magnetite and cerium dioxide. Magnetic properties (Figure 1) are characteristic of nanosized particles of magnetite.

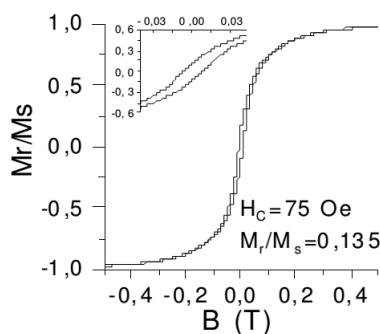


Figure 1. Hysteresis loops of Fe_3O_4 / CeO_2 .

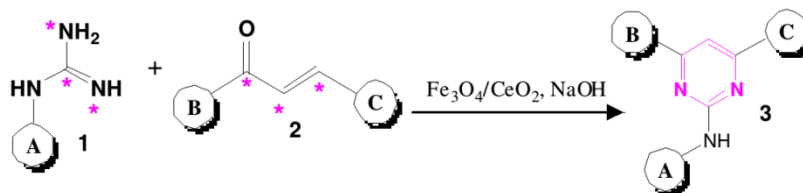


Figure 2. The reaction [3 + 3] of condensation with the present of Fe_3O_4 / CeO_2 nanocatalyst.

For the synthesis (Figure 2) of key pyrimidine amines 3, we used the reaction [3 + 3] of condensation of bis-electrophiles – arylguanidines 1 and bis-nucleophiles (substituted chalcones 2), forming a $\text{C}^4\text{--C}^5\text{--C}^6$ fragment of the pyrimidine ring, which proceeds efficiently in the presence of a Fe_3O_4 / CeO_2 nanocatalyst. Using a new nanocatalyst, the yield of target 2-aminopyrimidines increased from 25 – 30 to 68 – 80 %, the reaction time decreased by 2 times to 3 – 4 h.

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SCATTERING OF CHARGE CARRIERS ON PRISTINE AND MODIFIED BY ADSORPTION SURFACES OF EPITAXIAL Bi(111) NANOFILMS

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We present a review of UHV electric, magnetotransport ($T \approx 10$ K) and structural (LEED) experiments with crystalline Bi (111) nanofilms, possessing strong spin-polarized surface electronic bands (Rashba splitting), which were grown in situ on Si (111) substrates [1 – 5]. Varying the pristine film thickness d (between 20 and 100 bilayers), temperature and magnetic field, we disentangled two transport channels. One remains indeed metallic at all thicknesses investigated and exhibits a slightly increasing conductance as a function of d , whereas the second is activated with a d -dependence of the activation energy, indicating a quasi-harmonic confining potential. Both channels reflect the electronic properties of the entire film and do not allow us to strictly separate surface and bulk states. While there is clearly no bulk conductivity, the activated channel is consistently described as electronic excitation into the partly occupied quantum well states, which are also responsible for the metallic conductance and preferentially located close to both interfaces of the film [1].

Measuring magnetoconductance and the Hall effect, we examined the scattering of surface spin-polarized conduction electrons on magnetic (Cr [2], Tb [3], Fe and Co [4]) and non-magnetic (Bi [2], Pb, Sb) impurities adsorbed on Bi (111) nanofilms. Individual 3d magnetic adatoms were found to be the most efficient scatterers exhibiting strong spin-orbit scattering. Details of chemical bond formation for impurities, particularly charge transfer between the adatoms and Bi surface, were shown to be crucial for local spin moments and electronic scattering properties.

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CELL POLARITON: A QUANTUM STATE IN THE MYELIN SHEATH OF NERVE

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Various polaritons are arousing tremendous interests in physics and material sciences for their unique and amazing properties, especially including the condensation, lasing without inversion and even room-temperature superfluidity.

Here, we propose a cell polariton (CP): a collectively coherent mode of a photon and all phospholipid molecules in a myelin sheath formed by glial cells. CP can be resonantly self-confined in the myelin sheath under physiological conditions (**Figure 1**). The observations benefit from the specifically compact, ordered and polar thin-film structure of the sheath, and the relatively strong coupling of the mid-infrared photon with the vibrons of phospholipid tails in the myelin.

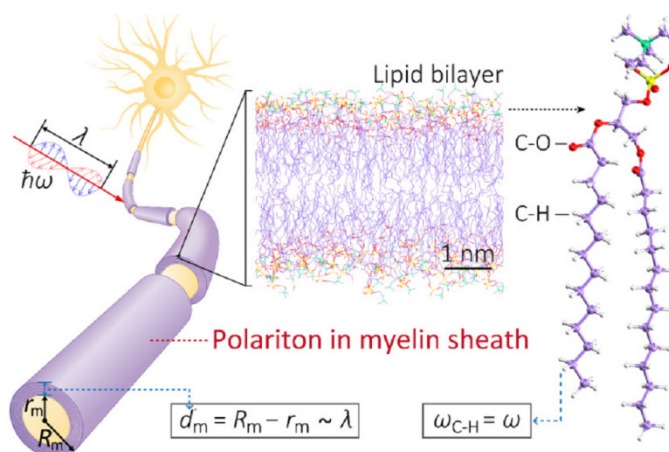


Figure 1. Cell-polariton resonantly and coherently forming in myelin sheath.

The underlying physics is revealed to be the collectively coherent superposition of the photon and vibrons, the polariton-induced significant enhancement of myelin permittivity, and the resonance of the polariton with the sheath cell [1].

Our findings provide the new understanding of high-efficient energy utilizations by neural cells, as well as a potential way for the designing of super-efficient energy materials and devices.

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HYBRID P3HT : PCBM / GaN NANOWIRES / Si CASCADE HETEROJUNCTION FOR PHOTOVOLTAIC APPLICATIONS

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Poly(3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) are commonly used for the fabrication of bulk heterojunction (BHJ) solar cells. However, power conversion in organic photovoltaics (OPV) is limited by low electrical performance of organic layers and high recombination rate. Efficiency limitations of organic solar cells could be circumvented by addition of inorganic nanostructures [1]. Also, integration of organic blends with well-developed silicon photovoltaic technology is ultimately desirable.

In this study hybrid cascade heterojunction in P3HT : PCBM / GaN NWs / Si architecture have been fabricated. P3HT : PCBM organic blend was spun onto GaN nanowire ensembles synthesized on monocrystalline silicon by molecular beam epitaxy. 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. Characteristics of P3HT / GaN hybrid heterojunction were calculated from Mott-Schottky measurements.

Addition of nanowires led to improvement in photovoltaic performance. Open circuit voltage has risen by 72 % and short circuit current density by 200 % compared to similar flat-architecture devices. Series resistance has decreased 50 times and power conversion efficiency has risen 20.7 times. Additional maxima are found in photocurrent spectrum corresponding to carriers being generated near GaN absorption edge. Moreover, External Quantum Efficiency peaks near GaN absorption edge, indicating the formation of current transfer channel via P3HT / GaN / Si cascade heterojunction.

Results obtained are useful for understanding of physical processes occurring in hybrid bulk heterojunction structures with nanostructured electrode.

Financial support: Polish National Science Center Grant: 2016/21/B/ST5/03378.

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NANO SILICA, AND PDMS LOADED HYDROPHOBIC, AND SUPERHYDROPHOBIC COATINGS FOR THE PROTECTION OF CALCIUM CARBONATE STONES

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Natural stones are continuously weathered due rain, wind and atmospheric gases. Water is one of the most significant causes of the deterioration of stone because it causes weathering due to atmospheric pollutants, disintegration inside and on the surface of the stone, cracking through freezing-thawing or wetting-drying cycles and salt crystallization inside the pores. Moreover, water aids in the growth of microorganisms and the formation of crusts [1]. Therefore, it is very important to develop hydrophobic coatings for the protection of natural stones.

One of the methods of developing hydrophobic coatings for stones is the sol-gel method. Incorporating organic PDMS into inorganic silica network can form flexible and hydrophobic coatings. Nanopowders can further increase this hydrophobicity both by adding roughness [2], and also by their intrinsic hydrophobicity, if they are hydrophobically modified.

In this research, we developed organic-inorganic hybrid hydrophobically modified nano silica (% 1 w/w) and PDMS loaded hydrophobic and superhydrophobic coatings for the protection of calcium carbonate stones by the sol-gel method, and analyzed the effect of the amount of PDMS (% 5, 10, 20, 30 w/w with respect to the alcohol content) on the hydrophobicity of each coating by measuring the contact angle values of the coated calcium carbonate samples and correlated these results with AFM measurements, and SEM images. We exposed the coated samples to humidity, and UV aging tests to evaluate the protective efficiency of the coatings, and compared these results with the commercial Silres BS 290 coating.

The results show that even though the optimum PDMS loading before the humidity test is % 10 in terms of contact angle, whereas after the humidity test, the optimum PDMS loading is % 30 which both have better performance than the commercial BS 290 coating. In terms of colorimetric properties, all of the as-developed and commercial coatings show superior performance both before, and after the UV aging test, and doesn't cause color change perceivable to the naked eye.

This work was funded by TUBITAK Marmara Research Center.

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MIRACLES OF CARBON ON THE NANOSCALE

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With its hybridization changing easily between sp^1 in carbon nanowires, sp^2 in graphitic carbon, and sp^3 in diamond, carbon takes a unique place in the periodic table [1 – 5].

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PROGRESS IN WATER DESALINATION: INSIGHT FROM *ab initio* STUDIES

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Whereas water itself is bountiful on Earth, much of it requires treatment to make it suitable for human consumption. Lack of potable water is currently the leading cause of death, ahead of any disease. Recent progress in fabricating nanostructured carbon allotropes may bring a long-awaited paradigm shift in designing membranes that would make efficient desalination of salt water using reverse osmosis and filtration of contaminated water possible.

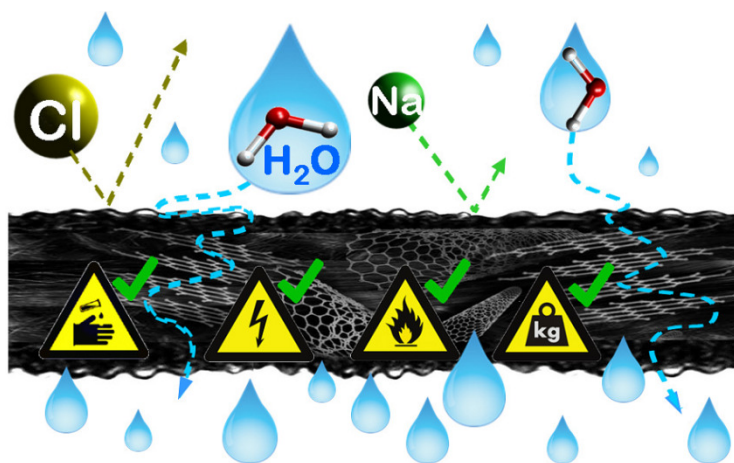


Figure 1. Design and advantages of an all-carbon membrane for water desalination and filtration.

A previously unexplored membrane design [1] based on a unique layered assembly (Figure 1) of carbon nanostructures including graphite oxide (GO), buckypaper consisting of carbon nanotubes, and a strong carbon fabric should provide high mechanical strength and thermal stability, resilience to harsh chemical cleaning agents and electrical conductivity, thus addressing major shortcomings of commercial reverse osmosis membranes. Microscopic insight into the critical permeation of water molecules in-between GO layers and across in-layer vacancy defects in graphitic carbon can be obtained using *ab initio* density functional theory calculations.

Results of these computational studies elucidate the reason for selective rejection of solvated Na⁺ ions in an optimized layered all-carbon membrane.

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LOW TEMPERATURE MAGNETIC PROPERTIES OF SOLID SOLUTIONS BASED ON LANTANUM INDATATE

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When considering the magnetic properties of materials, only the contributions of ferro- or paramagnetic ions are usually taken into account. The contribution of diamagnetic ions is usually neglected. However, for magnetically diluted materials containing small amounts, for example, of paramagnetic particles, one can expect that the contribution of diamagnetism may be comparable with the contribution of paramagnetic particles and even exceed it (especially at low temperatures). Only a few cases of experimental verification of this assumption are known. In this work, an attempt is made to compare the contributions of dia- and paramagnetic ions to the magnetic properties of ceramic samples of $\text{La}_{1-x}\text{Ln}_x\text{InO}_3$ solid solutions ($\text{Ln} = \text{Pr}, \text{Sm}, \text{Eu}, \text{Nd}$; $x = 0.001 - 0.1$).

It was found that the specific magnetization (σ_{sp}) of the majority of the studied solid solutions with increase of the magnetic field (up to 14 T) increases nonlinearly with a gradual approach to magnetic saturation, which, however, is not achieved in a field up to 14 T.

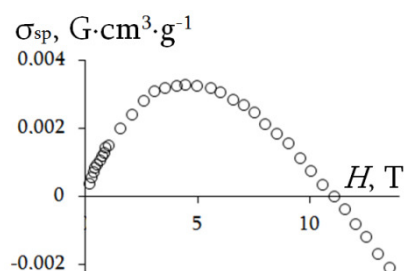


Figure 1. Field dependence of the specific magnetization of $\text{La}_{0.995}\text{Eu}_{0.005}\text{InO}_3$ at 5 K.

At 5 K for $\text{La}_{0.995}\text{Eu}_{0.005}\text{InO}_3$ (**Figure 1**) and $\text{La}_{0.999}\text{Pr}_{0.001}\text{InO}_3$, an increase of the magnetic field up to 5 T leads to a gradual increase of the paramagnetic specific magnetization. With a further increase of the magnetic field, a gradual decrease in the value of the specific magnetization occurs, which then passes into the negative (diamagnetic) region. This is due to the fact that the diamagnetic contribution to the magnetization of these solid solutions becomes larger than the paramagnetic one, and in magnetic fields above 11 T it is determined by the diamagnetic contribution. Specific magnetization at 5 K of other solid solutions based on lanthanum indatate is positive in magnetic fields up to 14 T. Undoped LaInO_3 is diamagnetic in magnetic fields up to 14 T. Thus, the results of this work indicate that in the case of dilute magnetic materials, the diamagnetic contribution to the magnetization of the samples can indeed prevail over the paramagnetic contribution.

SUPERCritical PROCESSING OF NANOMAGNETIC POLYMER COMPOSITES

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Supercritical carbon dioxide (SCC) has received growing attention over decades as benign medium for synthesis and modification of polymer. Unique combination of pressure tunable density, viscosity and diffusivity allows SCC to serve as environmentally benign medium for filler dispersion, polymerization reactions and polymer modification [1, 2]. Present study demonstrates a novel method of processing of epoxy based nanomagnetic polymer composites (NPCs) through SCC assisted diffusion of epoxy resin (ER) into magnetic domains of siliconized ferrofluid (SF) at 90 °C, 1200 psi, followed by curing.

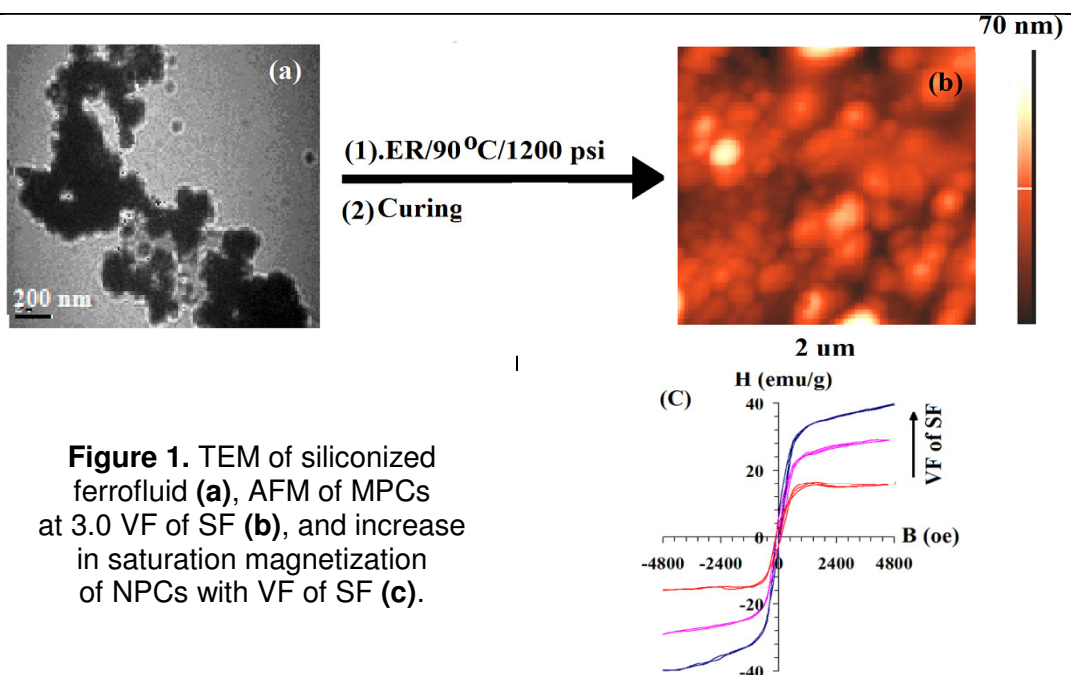


Figure 1. TEM of siliconized ferrofluid (a), AFM of MPCs at 3.0 VF of SF (b), and increase in saturation magnetization of NPCs with VF of SF (c).

Atomic force microscopy, X-ray diffraction, four probe DC conductances and magnometry reveals dispersion of nanomagnetic domains into epoxy matrix (**Figure 1**). With volume fraction (VF) of SF, ranging 1.0 to 3.0 into ER, the saturation magnetization (emu/g) of NPCs was increase ranging 15.65 to 39.50. NPCs derived at 2.0 VF of SF has rendered increase in Rockwell hardness by 16 % with simultaneous rise in their wear resistance up to 28.5 % at 4 bar and 230 rpm. With VF of SF, the compressive and impact strength of NPCs were improved (%) to 21.0 and 45 with a marginal compromise in their tensile strength and thermal stability. NPCs has shown DC conductance of $0.85 \cdot 10^{-3}$ S/cm with percolation threshold at 2.0 VF of SF.

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DIMENSIONAL AND TEMPERATURE DEPENDENCE OF THE ELASTIC MODULUS

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To study the dependence of the elastic modulus on the dimensional factor of the material and temperature, some methods have been developed for estimating: (a) the energy of the external surfaces of the samples and taking into account their influence on the internal state of the electron–ion system; and (b) the values of the melting temperature of the material (single-phase and two-phase) depending on the size.

A method is proposed for estimating the energy of the samples external surfaces and for taking into account their influence on the internal state of the electron–ion system. The temperature dependences of the elastic moduli of materials (metals, high-entropy alloy, ceramic materials, borides, nitrides, dielectrics, eutectic systems, etc.) are calculated from the first principles and analytically presented with taking into account the size factor [1]:

$$E_d(T) = E_0 \left(1 - \frac{K_p}{d} \right) \left(1 - \frac{0.2T}{T(d)} - \frac{0.25T^2}{T^2(d)} \right).$$

Here E_0 is the Young's modulus of bulk material, $T(d)$ is the melting temperature of the material depending on the size. **Figure 1** shows the temperature dependences of the normalized Young's modulus $E_d(T)/E_0$ on the temperature and size of the materials.

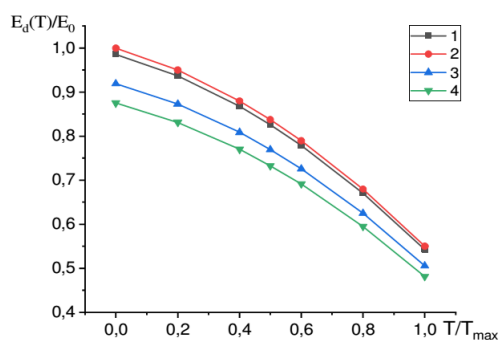


Figure 1. Dependence of the normalized Young's modulus $E_d(T)/E_0$ on $T/T_{\max}(d)$ for different values of the plate thickness d for: (1) bulk LaB₆ material, (2) LaB₆ nanoplates with a thickness $d = 5$ nm, (3) for the LaB₆–TiB₂ system with thickness $d = 10$ nm, and (4) LaB₆–TiB₂ with thickness $d = \text{nm}$.

The obtained analytical formulas have significant practical value. These formulas make it possible to obtain the elastic modulus of different materials (metals, HEAs, semiconductors, dielectrics, borides, carbides, nitrides and eutectic quasi-binary composites based on metals, carbides, borides, etc.) depending on the temperature and size of the plate thickness, at the presence of basic parameters of the bulk materials under study (lattice parameter and elastic modulus).

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VIOLET PHOSPHORUS AND PHOSPHORENE

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Black phosphorene has attracted much attention as a semiconducting two-dimensional material. Violet phosphorus is another layered semiconducting phosphorus allotrope with unique electronic and optoelectronic properties. However, no confirmed violet crystals or reliable lattice structure of violet phosphorus had been obtained. Now, violet phosphorus single crystals were produced and the lattice structure has been obtained by single-crystal X-ray diffraction to be monoclinic with space group of $P2_1/n$ (13) ($a = 9.210 \text{ \AA}$, $b = 9.128 \text{ \AA}$, $c = 21.893 \text{ \AA}$, $\beta = 97.776^\circ$). The lattice structure obtained was confirmed to be reliable and stable.

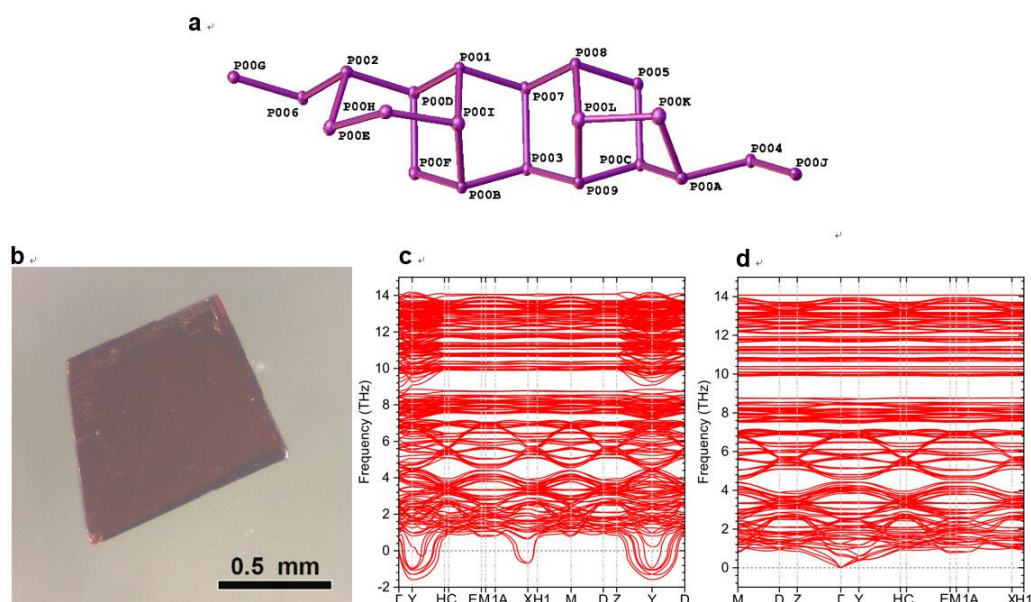


Figure 1. The crystal structure of violet phosphorus: **(a)** minimum asymmetric unit; **(b)** optical microscope image of a violet phosphorus single crystal; **(c)** the phonon dispersive curves of violet phosphorus; and **(d)** our violet phosphorus in the Brillouin zone.

The optical band gap of violet phosphorus is around 1.7 eV, which is slightly larger than the calculated value. The thermal decomposition temperature was 52 °C higher than its black phosphorus counterpart, which was assumed to be the most stable form. Violet phosphorene was easily obtained by both mechanical and solution exfoliation under ambient conditions. Results are briefly summarized in **Figure 1**.

PAIRING TRANSITION IN INTERACTING ELECTRONIC DOUBLE LAYERS

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In a system of two parallel two-dimensional layers we study the pairing transition caused by interlayer Coulomb interaction. Depending on the charge carriers, which can be electrons or holes, the interaction is either repulsive for two electron layers or attractive for an electron and a hole layer. In the latter case the paired state consists of excitons [1] while in the former case we get electron pairs [2]. It is important that these two pairing states are related by a duality transformation.

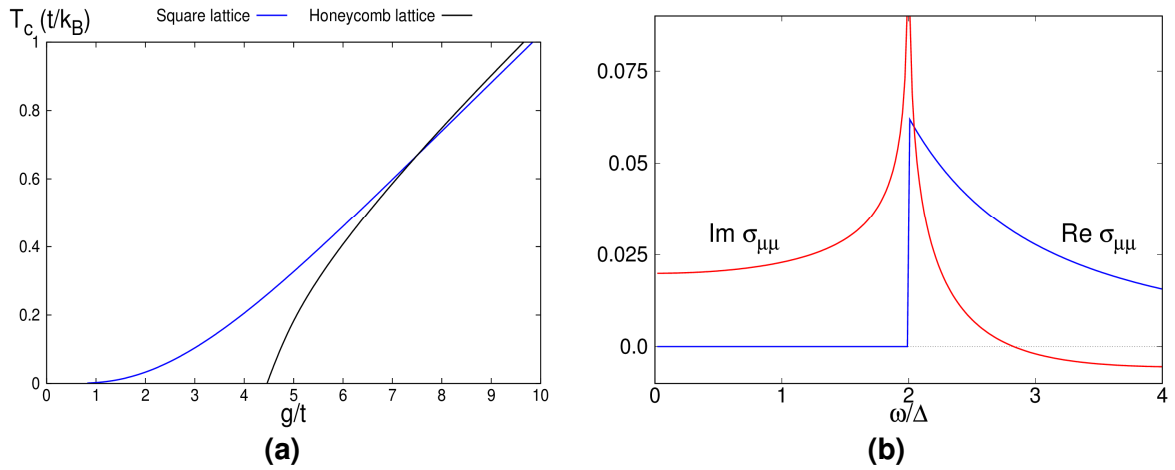


Figure 1. Critical temperatures for a square lattice and a honeycomb lattice as a function of the interaction strength g (a); and optical conductivity of frequency ω describes the Coulomb drag (b).

The pairing transition depends on the density of states and requires a critical interaction strength in the case of a honeycomb lattice, where the density of states vanishes at the Fermi energy (**Figure 1a**). The paired states have a characteristic behavior in terms of the optical conductivity, which reflects the Coulomb drag effect (**Figure 1b**).

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