GEORGIAN TECHNICAL UNIVERSITY

4th International Conference “Nanotechnologies”

October 24 – 27, 2016, Tbilisi, Georgia

Nano – 2016

ABSTRACTS

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ABSTRACTS

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This abstracts book includes about 210 abstracts of papers presented at the 4th International Conference “Nanotechnologies”, October 24 – 27, 2016, Tbilisi, Georgia (Nano – 2016) by professors and scientists of many leading universities and other research centers from more than 30 countries.

Compilers:

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SELF-PROPAGATING HIGH-TEMPERATURE SYNTHESIS OF BORIDE CONTAINING COMPOSITES

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Self-propagating high-temperature synthesis (SHS) has been used to prepare many refractory materials such as carbides, borides, silicides, oxides, hydrides, intermetallics and complex composites [1, 2] Transition metal borides are of special interest due to their unique physical-chemical properties and are widely used as the most promising materials in many branches of engineering, machine building, electronics, power industry [3]. However, strong covalent bonds inherent to phases of pure diborides of transition metals lead to low plasticity and low strength, thereby limiting the field of their use to a great extent. In this connection, at present great attention is paid to the technology of production of multicomponent composition materials containing metal borides in combination with more plastic materials playing the role of a binder. These can be, for example, aluminum or magnesium oxides which play the role of a high temperature binder and filler decreasing the content of expensive diboride, when producing composition materials [3, 4].

The aim of this study is SHS composite materials based on borides of titanium, chromium, zirconium using borate ore of Inder deposite of the Republic of Kazakhstan. SH-synthesis was carried out in the systems TiO_2–B_2O_3–Al, Cr_2O_3–B_2O_3–A1, $ZrSiO_4$–Al–B_2O_3, (where B_2O_3 is in the composition of borate ore). Samples were prepared from the charge containing titanium, chromium oxides, aluminum, borate ore of Inder deposit (the content of boron oxide up to 40 %), natural mineral-zirconium $ZrSiO_4$. Preliminary mechanical activation was carried out in a high power planetary-centrifugal mill. The microstructure and phases composition of synthesized products were investigated using microanalyses-scanning electron microscope JCXA–733 (JEOL) “Superprobe” and Hitachi S–4800 FE–SEM, Japan and XRD. The prepared samples were burnt at room temperature in air initiating ignition by magnesium.

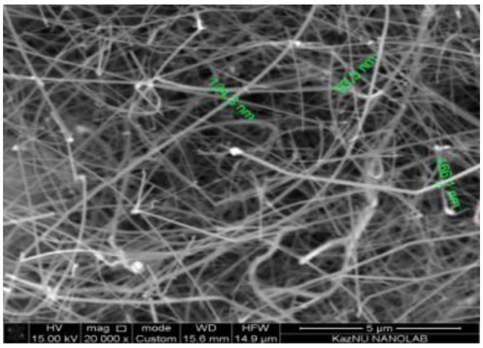

Figure 1. The microstructure of SHS products of the system $ZrSiO_4$–Al–B_2O_3.

Investigation of the microstructure of the compositions revealed the formation of whiskers of aluminum oxide with length of about 10 – 25 µm and with diameter of 50 – 200 nm (**Figure 1**). The possibility of using borate ore of Inder deposite for synthesis of refractory composite is shown.

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FEASIBILITY STUDY ON THE USE OF Gen5 PECVD REACTORS FOR MANUFACTURING OF HIGH-EFFICIENCY SILICON HETEROJUNCTION SOLAR CELLS

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G. Ivanov [1], I. Nyapshaev [1], D. Orekhov [1], A. Semenov [1], I. Shakhray [1],
G. Shelopin [1], E. Terukov [1], B. Strahm [2], G. Wahli [2], P. Papet [2],
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In this study we evaluate the potential of using Gen5 (1.4 m^2) KAI PECVD reactors, originally designed for production of thin film silicon modules, for manufacturing of high-efficiency silicon heterojunction (Si–HJ) solar cells. It is shown that Gen5 KAI PECVD reactors can provide an excellent uniformity of optical and electrical properties of hydrogenated amorphous silicon layers across entire surface of a 110 × 130 cm^2 wafer carrier. Surface passivation with low surface recombination velocity (< 4 cm / s) is achieved on n-type FZ c-Si wafers. Si–HJ solar cells, with an efficiency as high as 20.4 %, are produced using commercial 6 inch n-type CZ c-Si wafers and Gen5 KAI PECVD reactors. The potential to reach the efficiency above 21 % is also demonstrated.

X-RAY SCATTERING STUDY OF THE PROPANOATE ESTER OF HYDROXYPROPYL CELLULOSE IN THE LIQUID CRYSTAL STATE SUBJECTED TO SHEAR FLOW

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The development of a global preferred orientation in the thermotropic phase of the propanoate ester of hydroxypropylcellulose subjected to shear flow is evaluated using time-resolving X-ray scattering procedures. At low shear rates the global orientation parameters, <P2>, <P4>, are close to zero, but at a critical shear rate which shows some dependence on the temperature, there is a marked increase in orientation with shear rate. However, a flow aligning regime is not attained for the shear rate range considered here (from 0.1 to 190 s^{-1}). Upon cessation of shear flow, the system relaxes to a globally isotropic state with a rate which is independent of the prior shear rate but is strongly dependent on the temperature.

EFFECT OF Cu DOPING ON STRUCTURAL AND SOME OPTICAL STUDIES OF NANO NiO FILMS PREPARED BY SOL–GEL TECHNIQUE

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This research deals with the study of the structural and optical properties of as deposited pure NiO and Cu doped NiO nano films with various compositions (0.01, 0.05, and 0.1 mol %). NiO nano films of 100 nm thick were deposited on ultrasonically cleaned glass substrates by sol–gel spin-coating technique with the spin speed and spin time of 3000 rpm and 30 s, respectively. XRD results indicated that the films are polycrystalline and have cubic structure with a preferred orientation along (111). The average grain sizes of the crystallites estimated from XRD data was found to lie in the range of 19.11 – 26.21 nm. Data of AFM indicate that the surface of films is smooth.The optical transmittance value of nano NiO film reaches to 94 % in the VIS and NIR regions, while it is value of films deposited with 0.1 mol % Cu reaches to 92 % which is important for its applications as window layers in solar cells. The values of optical energy gap of NiO and Cu doping by 0.01, 0.05, and 0. 1 mol % were equal to 3.73, and 3.61, 3.49, and 3.42 eV, respectively.

NOVEL PREPARATION OF NANOFILM SUITABLE TO FABRICATION SOLAR CELL FROM Al–Ni–Cr ALLOY BY THERMAL EVAPORATION TECHNIQUE

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In this study, we prepare nanofilm from Al–Ni–Cr alloy at thickness of 9, 11, 18 nm by thermal evaporation technique. From scanning electron microscope (SEM) study, it can show that the films free from crystal defects like pin holes and cracks, homogeneous and smooth. From atomic force microscopy (AFM), it's found nanofilms, the root mean square decreased with increasing thickness, while thegrain size increased with increasing of thicknesses of the films from 24.01 nm at thickness of 9 nm to 63 nm at thickness of 30 nm. The optical measurement shows that the Al-Ni-Cr nanofilms transmittance decreases with increasing of thickness, the energy gap decreased from 2.2 eV for film thickness 9 nm to 0.7 eV for film thickness 30 nm, that refer to convert the conducting alloy to semiconductor at small thickness (less than critical thickness). Hall measurements showed that all the films are n-type and carrier concentrations increases with increasing thickness, carrier concentrations and mobility are increases with increasing of thickness. The resistivity decreased with increasing film thickness from $1.216 \cdot 10^2$ $(\Omega \cdot \text{cm})^{-1}$ for 18 nm thickness to $1.268 \cdot 10^5$ $(\Omega \cdot \text{cm})^{-1}$ for 9 nm thickness.

COMPARISON OF SYNTHESIS METHODS OF MAGNETIC NANO–PARTICLES AND THEIR EXPERIMENTAL CHARACTERIZATION

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Ferrofluids consist of magnetic particles of submicron sizes dispersed in liquid carrier and stabilized against agglomeration and sedimentation by appropriate coating. In non-polar carriers the most common agents are surfactant molecules with long alkyl tails. They form a surfactant shell around the particles which provides steric repulsion between them, and prevents their agglomeration. For technological purposes the main task is to obtain ferrofluids with well dispersed particles, and with controlled sizes and size distributions. Such systems are commonly available now, and various synthesis methods are worked out and used successfully. The main factors affecting the behavior of a given ferrofluid are the mean particle size, concentration and the polydispersity. These parameters can be tailored by choosing the appropriate synthesis route. Dispersions of magnetite and mixed ferric oxide particles of about 10 nm sizes have been prepared using different methods of synthesis: aqueous co-precipitation of iron salts, thermal decomposition of metal complexes, and mechanical grinding of large grain magnetite powders. We explore the differences between ferrofluids prepared by different methods, such as particle morphology, their interactions, and the overall structure of the colloids. The extremely small sizes limit the accuracy of all structure-sensitive experimental methods. Often the quantitative differences between the results obtained by various methods are significantly larger than the experimental errors, estimated from the data treatment. The reasons of these discrepancies will be discussed. The methods of nanoparticle morphology analysis may be divided into two general groups. The first group is associated with detection of individual nano-objects, such as the electron microscopy, or atomic force microscopy. In the second group – magnetometry, X-ray diffraction, small-angle neutron and X-ray scattering – the integral response of a large ensemble of particles is detected. The data are usually analyzed by assuming certain models for the distributions of the physical properties of the particles, and the characteristic parameters of these distributions are obtained by e.g. numerical fitting procedures. We present results for twelve ferrofluids in aqueous and oilycarriers, compare the performance of each characterization technique and discuss some critical issues arising in experimental characterization of nanoparticles. The analysis and comparison of the collected data allowed us to assess the performance of each technique for obtaining precise structural data for dispersions of nanoparticles.

ADVANCED AND NANOMATERIALS: CHALLENGES AND OPPORTUNITIES

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This presentation will discuss the manufacturing process and applications of advanced and nanomaterials. It provides an overview of challenges in the manufacturing, formulation and scale up. Case studies and examples will be given for electronic, and energy materials. The opportunities and the pitfalls in developing these materials will be also discussed.

THEORETICAL STUDY OF THE ADSORPTION PROPERTIES OF POROUS BORON NITRIDE NANOSHEETS

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Experimental and theoretical studies of an h-BN hexagonal boron nitride monolayer, and some layered structures based on it, at the moment are of great interest due to its unique properties, as well as a variety of possible applications. One of the major goals in environmental protection is a high-efficiency cleaning of water resources from various contaminants. Some high-porous layered nanomaterials based on h-BN have been recently developed, they have excellent adsorption properties for oils, solvents and dyes [1, 2].

In this paper, we studied the adsorption of water, ethanol, ethylene glycol, and toluene molecules on the ordered h-BN sheet surface and a vacancy-containing sheet surface. We provide a comparison between the processes of interaction of the single molecules and their water associates with the ordered and porous cluster surfaces. This paper addresses the physical and chemical principles of water purification from organic contamination using hexagonal boron nitride with vacancy and multivacancy defects.

We used the $B_{48}N_{48}H_{24}$ clusters as a model system to simulate the one-layer hexagonal boron nitride nanostructures. Quantum-chemical simulation was performed using the semi-empirical schemes included in the MOPAC2012 software package [3]; unrestricted Hartree–Fock self-consistent field calculations and the PM6 approximation were done.

Analyzing the results of quantum-chemical calculations of the energy characteristics of molecule adsorption on the ordered hexagonal boron nitride and boron nitride containing a vacancy, it can be concluded that the existence of a vacancy defect leads to a significant chemical activity of boron nitride. In the defect area the possibility of strong covalent binding the atoms of nitrogen or boron with the fragments of the adsorbate molecules dissociation can be occur. However, the explanation of the physical and chemical principles of water purification by means of porous hexagonal boron nitride, in our opinion, is based on the adsorption of molecules from an aqueous solution (from the associates with the water molecules) on the partially passivated areas of vacancies and multivacancies (pores). Partial passivation induces the appearance of some single adsorption sites (one atom with a dangling bond) remaining in the area of a vacancy or multivacancy. It does not cause dissociation of an adsorbate molecule and thus its lasting and irreversible binding to hexagonal boron nitride. Therefore, single adsorption centers provide a possibility for adsorption of molecules (the supposed organic contaminants) from the aqueous solution, resulting in the bound states with a small binding energy that allows to restore a clean h-BN surface, for example, by annealing.

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ANTIREFLECTIVE AND HYDROPHOBIC COATED LENSES FOR PHOTOVOLTAIC MODULS

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An energy conversion efficiency of a solar cell as well as a quality of a lens concentrator is of great importance in modern PV (photovoltaic) modules. Lens concentrators must provide maximum energy through to solar cell and must be resistant against water and water vapor. Utilization ofa reflection losses from the inner and outer surfaces of lens so that maximize photon energy thatgoes through to solar sell was the work's purpose.

Multilayer antireflective coated polymer lens with high adhesion was proposed. Good adhesion was achieved by the formation of solid layer on the surface of the lens by means of sinking and removing the lens in the liquid polysiloxanevarnish basin before layering with antireflective coatings. The width of the solid layer is adjusted with the viscidity of polysiloxanevarnish and selection of sinking and removal velocity of the lens in the basin. After removing the lens from the basin polysiloxanevarnish polymerization is done by thermal treatment that significantly increases the lens connection strength to the surface. polysiloxanevarnish possesses high elasticity, created surface does not get damaged from the contact with the environment and is resistant against scratches.

The lens concentrator is layered with antireflective coatings according to programed computer calculations. Layering of the coatings is performed in a vacuum chamber by forming the solid layer. The width of coatings (several tens of nanometer) and consistency is defined by equipment with two identical planar magnetron emission magnetrons. Both sides of the lens concentrator are deposed, first with low refraction indicator (first layer SiO_2, $n = 1.45$), and then on the surface of the first layer the second layer with high refraction indicator is applied (ZrO_2, $n = 1.98$). By reiterating of these layers in rotation the antireflective coating is created.

Hydrophobic coatings on the antireflective layer are formed to provide sustainability against water and water vapor. Once again basin sinking method is used. Basin solution in this case was the specific viscid solution made from ftoroplast powder. Sinking and removal velocities of lens remain unchanged compared to the previous processes. Polymerization of hydrophobic coating of the lens concentrator is performed in a thermostat at temperatures 60 – 70 °C.

Hydrophobic coating produced by following the above method provides the protection of the lens surface from water and water vapor coercion and from formation of water. As they have low rate of friction the increased moisture angle is lowered with these vaporization.

On the basis of the technology described above we have manufactured lab models of lens concentrators intended for solar photoelectric converters. These samples have been tested with the spectrometer and established that the light intensity in spectral area 550 – 750 nm has increased at 8 % on average.

MAIN TYPES OF CONDENSED PHOSPHATES OBTAINED IN OPEN SYSTEMS FROM SOLUTION – MELTS OF PHOSPHORIC ACIDS

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The phosphorus chemistry has becoming increasingly important in 21th century following a number of recent scientific interdisciplinary researches and utilisation of advanced technologies. Particularly chemistry of condensed phosphates or that is to say inorganic polymers – developed much rapidly, for the causes of the development of advanced methods of analysis and of the significant application of phosphates materials in various domains including nanotechnologies. Among a varieties of processes of condensation of phosphoric anions one of them leads to the prearrangement of cyclic, oligomeric or polymeric structures of condensed phosphates [1, 2].Last decades we reported [3 – 5] about our studies in the open systems $M^I_2O–M^{III}_2O_3$ within temperature range 130 – 550 °C, where M^I are the alkali metals and M^{III} are Ga, In or Sc. Various experiments revealed the existence of the following double condensed compounds – in fact a series of a formerly new class of inorganic polymers (**Table 1**).

Table 1. Synthesized phosphates in systems $M^I_2O–M^{III}_2O_3–P_2O_5–H_2O$.

$M^IM^{III}(H_2P_2O_7)_2$	$M^IM^{III}P_2O_7$	$M^{III}H_2P_3O_{10}$	$M^IM^{III}HP_3O_{10}$ and / or other complex anions	$M^I_2M^{III}P_3O_{10}$	$M^IM^{III}(P_2O_3)_4$
$LiGa(H_2P_2O_7)_2$	$LiGaP_2O_7$	$GaH_2P_3O_{10}·H_2O$ Form I	$Li_xH_{2–x}GaP_3O_{10}·(1–1.0)H_2O$	$Li_2GaP_3O_{10}$	$(LiGa(PO_3)_4)_x$
$NaGa(H_2P_2O_7)_2$	$NaGaP_2O_7$	$GaH_2P_3O_{10}·H_2O$ Form II	$KGaP_3O_{10}$		$NaGaP_4O_{12}$
$KGa(H_2P_2O_7)_2$	$KGaP_2O_7$		$RbGaHP_3O_{10}$ Form I		$K_2Ga_2P_8O_{24}$
$RbGa(H_2P_2O_7)_2$ Form I	$RbGaP_2O_7$		$RbGaHP_3O_{10}$ Form II		$Rb_2Ga_2P_8O_{24}$
$RbGa(H_2P_2O_7)_2$ Form II	$CsGaP_2O_7$		$CsGaHP_3O_{10}$ Form I		$Cs_3Ga_3P_{12}O_{36}$
$LiIn(H_2P_2O_7)_2$	$LiInP_2O_7$		$CsGaHP_3O_{10}$ Form II		$LiIn(PO_3)_4$
			$CsGaHP_3O_{10}$ Form III		$NaInP_4O_{12}$
			$Cs_2GaH_3(P_2O_7)_2$		
$NaIn(H_2P_2O_7)_2$	$NaInP_2O_7$		$RbInHP_3O_{10}$		
$KIn(H_2P_2O_7)_2$	$KInP_2O_7$		$CsInHP_3O_{10}$		
	$CsInP_2O_7$				

The presented data are the result of experiments on synthesis and investigation of structure of an earlier unknown compounds – double condensed di- and triphosphates of scandium and silver: $AgSc(H_2P_2O_7)_2$, $Ag_2ScH_3(H_2P_2O_7)_2$ and $AgScHP_3O_{10}$. The method of synthesis of double phosphates from solution – melts of phosphoric acids was applied.

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

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Graphene physics in our days opens large research field including low-energy condensed matter physics and quantum electrodynamics (QED) since quasiparticles states in graphene behave like massless "relativistic" Dirac fermions and obey a two-dimensional Dirac equation with the Fermi velocity much less than the light speed in vacuum [1]. These facts lead to significant applications of graphene in the fundamental nonlinear QED processes in the weak and moderately strong external electromagnetic radiation fields compared to superintense laser fields of ultrarelativistic intensities which are required for observation of vacuum nonlinear phenomena such as production of electron-positron pairs from the extremely intense laser beams, nonlinear Compton scattering, stimulated bremsstrahlung (SB) etc in the strong and superstrong radiation fields [2 – 4].

In the present work we develop the relativistic quantum theory of induced scattering of 2D Dirac particle on an arbitrary electrostatic field of impurity ion in the presence of an external electromagnetic radiation field (actually terahertz radiation to exclude the valence electrons excitations at high Fermi energies), taking into account the interaction with the scattering potential in the Born approximation. The scattering rates and total multiphoton cross-sections of SB of conductive electrons on the impurities in the doped graphene at the presence of moderately intense radiation field have been obtained. The analytic formulas in case of screened Coulomb potential have been analyzed numerically for actual parameters of interaction system in the strong radiation field. We have investigated the angular dependence of scattered Fermi electrons for large range of radiation intensities. It is shown that the strong coupling of massless quasiparticles in the quantum nanostructures to a strong electromagnetic radiation field leads to the strongly nonlinear response of graphene which opens diverse ways for manipulating its electronic transport properties by coherent radiation fields.

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LANDAU-QUANTIZED GRAPHENE IN STRONG RADIATION FIELD AND HIGH HARMONIC GENERATION

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Due to the exotic nonlinear electromagnetic (EM) properties of graphene [1], it is extensively considered as an active material for diverse nonlinear optical applications [2]. Thanks to unusually high interaction parameter with EM radiation field, the graphene is an effective material for multiphoton interband excitation, wave mixing and high harmonic generation (HHG) processes [3 – 6]. When a static uniform magnetic field is applied perpendicular to the graphene plane, the electron energy is quantized forming nonequidistant Landau levels. As a consequence, in the graphene the anomalous quantum Hall effect takes place [7]. Under these circumstances the main works have concentrated on the static or linear optical properties of the Landau-quantized grapheme. Meanwhile, it is important the exploration of nonlinear response of Landau-quantized graphene to a strong coherent radiation. As was shown in [8], the nonlinear optical response of graphene to a moderately strong laser radiation in the quantum Hall regime, in particular, third harmonic intensity and nonlinear Faraday effect have a characteristic Hall plateau structures that persist for a wide range of frequencies and intensities even for significant broadening of Landau levels because of impurities in graphene. Due to the peaks in the density of states one can also expect enhancement of high harmonic radiation power of Landau-quantized graphene. Hence, it is of interest to consider HHG process in the ultrastrong wave-graphene coupling regime. 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 study of nonlinear phenomena in condensed matter physics is important.

In the present work, a microscopic theory of the Landau-quantized graphene interaction with strong coherent EM radiation is presented. The results of our investigations show that one can achieve efficient yield of HHG with strong radiation fields – when the work of the wave electric field on the magnetic length is much larger than pump photon energy. At that for the specific frequencies and gated level one can achieve considerable enhancement of HHG rate.

This work was supported by the State Committee of Science MES RA, in the frame of the research project # SCS 15T–1C013.

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PREPARATION AND CHARACTERIZATION OF A NOVEL GELATIN/NANODIOPSIDE/NANOHYDROXYAPATITE COMPOSITE SCAFFOLDS FOR TISSUE ENGINEERING APPLICATIONS

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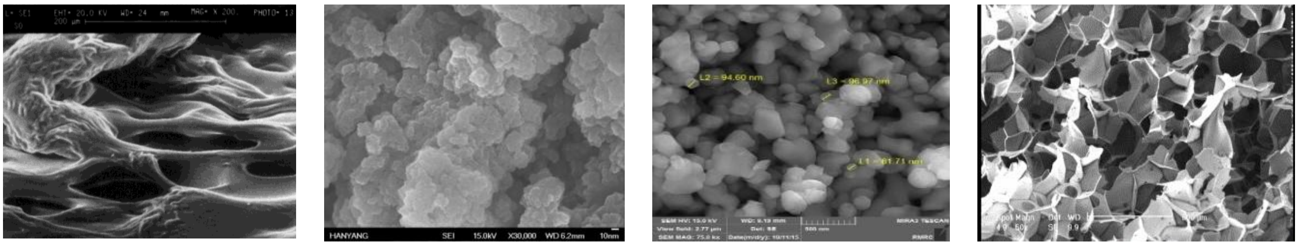
Gelatin/nanodiopside/nanohydroxyapatite (GE/nDP/nHAp) composite scaffolds were prepared from the mixture of GE, nDP and nHAp in different inorganic/organic weight ratios by using the freeze–drying method [1 – 3]. The prepared nHAp, and composite scaffolds were investigated using BET, FT–IR, SEM, and XRD techniques (**Figure 1**). The composite scaffolds had 70 – 85 % porosities with interlinked porous networks. Moreover, investigation of the cell proliferation, adhesion and viability using MTT test, and mouse preosteoblast cell proved the cytocompatibility nature of the composite scaffolds with improved cell attachment and proliferation. All these results essentially illustrated that this composite could be a potential for tissue engineering application.



b c d

a

Figure 1. SEM images of (a) pure GE, (b) pure nDP, (c) pure nHAp, and (d) composite 70 %.

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ULTRASONIC WAVES AND WATER PURIFICATION FROM NANOPARTICLES

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Ultrasonic wave as a high frequency sound wave effects on substances that refer toquantity and quality, and this property can be used in different fields. One of the most interesting applications is thermo dynamical property change of fluids by ultrasonic cavitation, which is possible to use for water purification of different unpleasant nanoscale particles [1]. Generally water treatment considered and compared with routine water treatment methods. Ultrasonic wave can be used as an alternative to produce pure water and some technical advantages of water treatment by ultrasonic waves comprised with the most common membrane method [2]. As sound waves travel, particles of medium vibrate more than common vibration then some physical properties of medium like density, temperature and pressure will change. These pressure changes divide into two parts as low-pressure and high-pressure regions. On the other hand, wave rhythm in fluid is depend on longitudinal wave rhythm [3]. Whenever ultrasonic wave as a high frequency longitudinal wave passes through liquid make acoustic cavitation, it forms fine bubbles in low-pressure region of fluid; because of pressure decrease then thermodynamic phase change of liquid to gas. Liquid atomizing effect, which produces the fine nanoparticles of liquid is the basis of the water purification. Ultrasonic atomizing process in practice is a little far from bubbles mathematical models because of different actual parameters effect in real conditions but in the range of particles size below 1 μm it is relevant. Despite of shifting to membrane method these days as a new method of water treatment, there are some conditional considerations that make thermal processes as the best choice specially when there is a source of heat energy, because the most important factor of thermal processes are thermodynamic water phase change. According to ultrasonic wave capability to make 0.01 – 0.5 MPa pressure and 2000 – 5000 K temperature, in practice, it can be significant as a new method of thermal water treatment. According to the data and analysis, acoustic cavitation by ultrasonic waves can be used as one of the most significant method of water purification [4]. Thermal processes not only can produce the clean purified water but also its quickness by high frequency and electrical fast controlling against slow mechanical systems make it more flexible in comparison to any other common method.

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ELECTRON-STIMULATED DESORPTION OF EXCITED ATOMS FROM NITROGEN FILMS

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Desorption or sputtering is among the most intensively studied radiation-induced phenomena. The term electron-stimulated desorption describes physical and chemical changes caused in the surface region of a solid by bombardment with low-energy electrons. Radiation effects in solid N_2 attract much attention in various areas of scientific researches including material and surface sciences, physical and chemical processes in interstellar space and solar system and also particle physics. Electronic desorption of solid nitrogen was studied under excitation with electrons, ions and photons [1]. Despite extensive studies, the contribution of excited atoms into the desorption is still not well understood.

In the present paper, radiation processes in the solid nitrogen irradiated with an electron beam were studied with special attention to the desorption of the excited atoms and its contribution to the electron-stimulated phenomena in general. The experiments were performed employing luminescence method and activation spectroscopy techniques – spectrally resolved thermally stimulated luminescence TSL and thermally stimulated exoelectron emission TSEE.

Atomic emissions were detected in the vacuum ultraviolet VUV range – the $^4P_{1/2–5/2} \rightarrow {}^4S_{3/2}$ transitions. They increased with respect to the bulk molecular emissions (the $A'^1\Sigma_u^- \rightarrow X^1\Sigma_g^+$ and the $A^3\Sigma_u^+ \rightarrow X^1\Sigma_g^+$) in thin films (< 100 nm) and under irradiation by slower electrons which have less penetration depth. Moreover, the observed atomic emissions coincided with the gas phase lines within the experimental error. These findings indicate the connection of the emissions observed with the desorbing excited atoms. Analysis of the spectrally resolved TSL and TSEE suggests connection of the atomic desorption with electron-ion recombination reaction. One can expect for the azide radical cation N_3^+ strong tendency to dissociate via N_2 + N channel. Formation of N radicals in the bulk of solid N_2 by this reaction was assumed in [2]. Thereby analysis of the VUV luminescence and relaxation emissions allowed us to observe formation of defects, dissociation of molecules into the atoms and the desorption of the excited atoms from the surface of solid nitrogen and also to define the electronic states of these atoms.

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THE EFFECT OF REDUCTION TEMPERATURE OF GRAPHENE OXIDE ON LOW TEMPERATURE ^{4}He SORPTION

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Graphene oxide (GO) is a material produced by chemical oxidation of graphite and subsequent exfoliation [1, 2]. This material is remarkable because it can be at least partly restored to the state of graphene sheets, resulting in the removal and recovery of oxygen-containing groups such graphene structure [2, 3]. The kinetics of sorption and subsequent desorption of ^{4}He gas by original graphite oxide (GtO) and thermally recovered samples of graphene oxide (TRGO, reduction temperature of 200, 300, 500, 700 and 900 °C) has been investigated in the temperature interval 1.5 – 20 K.When the temperature is lowered from 20 K to 11 – 12 K for all the samples was observed increasing in the time of sorption ^{4}He, it is typical for thermally activated diffusion. At temperatures below 5 K for samples GtO and TRGO–200 characteristic times of ^{4}He sorption weakly dependent on the temperature, it can be explained by the predominance of the tunneling mechanism of thermally activated diffusion. For samples of graphene oxide, the recovered heat at a higher temperature (300, 500, 700 and 900 °C), below 5 K was observed increasing ofcharacteristic times with decreasing temperature, which can be explained by the formation of defects in removing carbon planes oxygen containing groups. Estimating the activation energy of diffusion ^{4}He (Ea) showed that the treated sample at 200 °C, Ea decreases 2.9 times compared with the original graphite oxide sheets separation due to graphite oxide by evaporation waterintercalated between carbon planes. The nonmonotonic character of the dependence of Ea heat treatment temperature graphite oxide samples above 200°C is caused by two competing processes – reduction of carbon graphite structure that increases the activation energy and the formation of defects, lowering the activation energy due to the opening of additional surface areas and ways for sorption.

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PROSPECTS OF INDUSTRIAL APPLICATION OF NANOBORON AS A PROTECTIVE MATERIAL

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For their unique complex of physical, chemical and technological properties, materials based on nanostructured boron can have practically endless list of effective industrial applications.

Among them, specially important role is played by the boron-rich protective nanomaterials.

Here we consider some of them:

- anticorrosion coatings;
- protective coatings for steel tube bores;
- light-weight ballistic protection; and
- conformal (or even flexible) personnel body armor.

THE FLOW OF THE DC CURRENT THROUGH THE HIGH-TEMPERATURE SUPERCONDUCTING CERAMICS WIRES

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It is possible to represent the high-temperature superconducting (HTSC) ceramics in the form of josephson medium, or stochastic medium, formed by the superconductors granules with different parameters, during this the Josephson junctions are formed by the points of contacts between granules [1]. By averaging the Ginzburg–Landau equation in small volume containing a large number of granules, it was able to get the material equation [1] which relates averaged current density vector $\vec{j}$ and magnetic field vector potential. $\vec{A}$:

$$\vec{j} = -\frac{\vec{A}}{A}\frac{\rho a\pi}{8}\left[I_c\left(\frac{2\pi}{\phi_0}Aa\right)\exp\left(-\frac{\pi}{16}\left(\frac{2\pi}{\phi_0}Aa\right)^2\right) - \frac{a}{c}\left(\frac{1}{R}\frac{d\vec{A}}{dt} + C\frac{d^2\vec{A}}{dt^2}\right)\right],$$

where $\varphi_0 = 2.07...\times 10^{-7}$ G · cm^2 – magnetic flux quantum, c – light velocity, ρ – Josephson junctions concentration in the medium, I_c, R and C – mean values of the single junction critical current, active resistance and capacity, a – the average size of granules forming the josephson junction. It is obtained on the basis of above stationary equation that, the magnetic field penetrates into HTSC samples on the depth

$$\lambda_M = \sqrt{\frac{c\phi_0}{\pi^3 \mu I_c \rho a^2}},$$

where the value μ has the meaning of the magnetic permeability of the medium due to meissner currents of the individual granules only. It is shown by numerical simulation the magnetic field penetrates into the sample without forming the vortices in case the external magnetic field magnitude is not higher then

$$B_1 = 2.25676...\times\frac{\phi_0}{2\pi a\lambda_M}\cdot$$

The dependence of the critical DC value of the cylindrical wires from their diameters was also been defined using the numerical simulation of the stationary equation. Current flowing through the sample is concentrated mainly in the thin surface layer with thickness of around λ_M showing, thus, the skin effect on the direct current. As a result, the dependence of sample overall current from its diameter (for $D > \lambda_M$) has a character close to linear. Similarly, the dependence of the strip wire critical current from its width was investigated. Like for cylindrical wires, the current is concentrated in a narrow boundary layer with width of the order λ_M, thus conforming once again the presence of skin effect on direct current. The results obtained allow make the conclusion the skin-effect has a high significance appearing at low frequencies down to direct current in the high-temperature superconducting wires, consisting of a granular superconductors medium. Therefore, to achieve the highest possible currents flowing through the HTSC wire (both massive and strip), it seems appropriate to make them in the form of “litzendraht” or stranded wire consisting of a large number of not connected to each other strands with a thickness not more than a few λ_M. In the case of submicron and nanoscale superconducting granules width of unconnected conductors should be millimeter and submillimeter sizes.

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SYNCHROTRON-RADIATION PHOTOEMISSION STUDY OF THE Ba ATOMIC LAYER DEPOSITION ON MULTIFERROIC BiFeO$_3$

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Multiferroics are the novel group of materials exhibiting coexistence of magnetic and ferroelectric ordering. Magnetism and ferroelectricity are essential to many forms of current technology, and the queat for multiferroic materials, where these two phenomena are intimately coupled. Multiferroics have potential for applications in spintronics, data storage, sensors and in tuneable multifunctional devices. BiFeO$_3$ (BFO) is considered as the multiferroic with high Curie point of ~ 1100 K, and high Neel temperature of 643 K. BFO is characterized by relatively simple crystal structure as the rhombohedrally distorted perovskite. Recently, photoemission studies for the clean BFO have been carried out [1 – 3]. Most of BFO works focused on core level spectra. No study is devoted to the valence band spectrum and to the spectra of metal / BFO interfaces.

Data present first photoemission results obtained for the Ba ultrathin layer adsorbed on the ceramic BiFO surface and shown possibility of photoemission method to study effect of Ba adsorbtion on the electronic properties of multiferroics. We perform first photoelectron spectroscopy (PES) study of electronic structure of the ultrathin Ba/BFO interface. Experiments were carried out *in situ* at BESSY II, Synchrotron, Berlin, using PES with photon energies in the range of 80-900 eV. The normal photoemission spectra from the valence band (VB) and Bi 4*f*, O 1*s*, Fe 2*p*, and Ba 4*d* core levels were recorded.

An effect of Ba atomic layer deposition is found to induce a significant modification of the valence band and core level spectra that is originated from the strong interaction with the charge transfer between Fe, O, Bi surface atoms and Ba adatoms. The Ba adsorption on the BFO surface is found to cause significant change in the Fe $2p_{3/2}$ core level spectrum. As can been revealed, the atomic ratio of ions Fe^{2+} / Fe^{3+} is increased for Ba / BFO interface at Ba coverage near 1 ML. The new effect of Ba adsorption signifies the improving ferroelectric polarization. The Ba ultrathin layer on the BFO surface is found to produce the strong interaction between Ba adatoms and Fe ions in interface area. The Fe $2p_{3/2}$ core level evolution is obviously caused by the recharge between $Fe^{3+} \leftrightarrow Fe^{2+}$ ions and may be one of the reasons for enhanced ferroelectric and magnetic properties of BFO due to increasing in the amount of the Fe^{2+} ions.

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CARBON COATED ($Fe–Fe_3C$) AND Ag-DOPED LANTHANUM MANGANITE ($Ag_xLa_{1-x}MnO_3$) NANOCOMPOSITES FOR MAGNETIC HYPERTERMIA OF CANCER CELLS

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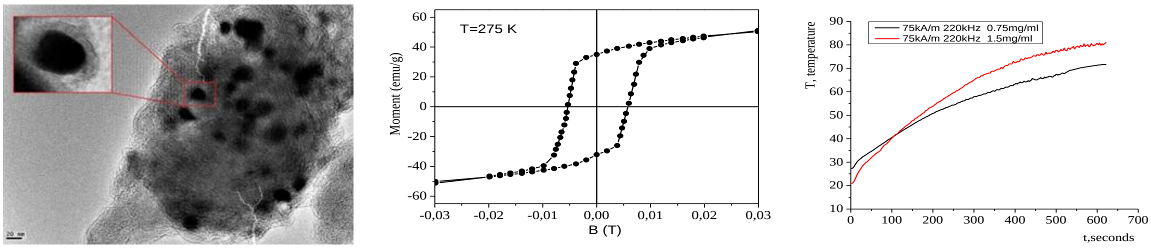
Carbon-coated ferromagnetic ($Fe–Fe_3C$) nanocomposites have been synthesized using solid-phase pyrolysis of metal-organic compounds. The structure, morphology and magnetic characteristics of these nanocomposites were investigated by electron microscopy, X-ray diffraction, Raman spectroscopy and magnetometry. The magnetic characteristics such as saturation magnetization and coercivity as well as the specific absorption rate (SAR) make these materials attractive for magnetic hyperthermia applications. Hysteresis loop of the ($Fe–Fe_3C$) & C nanocomposites is of special interest as it shows almost square behavior, where Mr / M (200 Oe) = 0.75. The limitation of the magnetic field amplitude and frequency $(H \cdot f) \leq 10.625 \cdot 10^6$ Oe / s makes this factor important that provides a high energy absorption even in case of low magnetic fields. The TEM image, hysteresis loop and heating saturations are shown in **Figure 1**.



(a) **(b)** **©**

Figure 1. TEM image (a), hysteresis loop (b), and experimental data of magnetic hyperthermia heating (c) for ($Fe–fFe_3C$) & C nanocomposites.

Ag-doped lanthanum manganite and carbon-black hybrids have been prepared by physical mixing of modified carbon and Ag-doped $LaMnO_3$ nanoparticles, followed by sintering at different temperatures. $Ag_xLa_{1-x}MnO_3$ nanoparticles were first synthesized via microwave enhanced chemical precipitation, and the carbon support was modified using graphitization, followed by HNO_3 and ammonia treatments. Microwave assisting yielded in improved uniformity of nanoparticles and reduced time of synthesis, which can become important for practical use of lanthanum manganite nanocomposites.

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LASER-INDUCED PERIODIC METAL STRUCTURES FOR SURFACE-ENHANCED SENSING

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Direct surface modification of materials using powerful laser pulses attracts more attention of researchers [1, 2]. Micro- and nanostructures on metal surfaces (copper and silver) have been obtained by the irradiation of the initial surface with Ti: sapphire femtosecond laser. The laser pulse with the wavelength of 800 nm, pulse duration of 130 fs, pulse energy around 0.8 mJ, repetition rate of 1 kHz focused on the surface with a long focal length lens. The change of the laser power density was achieved by changing the distance between the metal surface and the lens. Formed structures are promising for many important applications such as plasmonic emitters, biosensors, surface enhanced Raman spectroscopy (SERS), etc.

The morphology of metal surface has been studied with atomic force microscopy (AFM) and the scattering indicatrices analysis. Laser-induced surface periodic structures could be considered as quasi-periodic diffraction gratings with the period smaller than the wavelength of the laser radiation. The most probable mechanism of formation of these structures is associated with an interference of incident electromagnetic wave and surface plasmon polaritons (SPP) excited by the incident wave on the rough metal surface [3]. The evidence of the excitation of SPP on the laser-induced metal nanostructures has been demonstrated by the measurements of the specular reflectance spectra. Possibility of the field enhancement due to the resonant excitation of SPP has been realised by the effect of SERS of Rhodamine 6G dye (Rh6G) on obtained laser-induced Ag nanostructures.

Raman spectra of Rh6G adsorbed on laser-induced Ag structures and the non-treated Ag surface have been studied under different excitation wavelengths, and for different regimes of laser treatment. Raman spectra obtained under the excitation wavelength of 476.5 nm demonstrate greater Raman signal enhancement. From the analysis of the ratio of intensity of Raman bands [4] on structured and initial surface, the gain coefficient achieve a value up to 20. In this case, such behaviour proves that the dominant mechanism of SERS of Rh6G on formed laser-induced Ag nanostructure is electromagnetic mechanism that involves resonant excitation of surface plasmons.

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FORMATION OF COPPER NANOPARTICLES IN METASTABILE IRON ALLOYS

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The initial stages of degradation of the iron-based solid alloy, being oversaturated by a copper and having the structure of low carbon packet martensite, were investigated. The maximal durability of the martensite is reached after 425 – 475 °C release. Herewith, the contrast is observed at dislocations, which may be explained by formation of the zones enriched by the copper of about 5 nm in size.

The crystal structure of the zones is isomorphic to the matrix, but distorts it due to the lack of the size correspondence between Cu and Fe. It declines the mobility of dislocations tending to growth in durability of the martensite at the very early stages of degradation.

First clearly fixed effects related to ones possessing face-centered cubic lattice manifest themselves in the structure of the martensite at 500 – 550 °C release, i.e., when the partial decrease in durability follows the durability itself. Dislocations contain regularly arranged particles of the ejected phase of 5 – 10 nm in size.

At the micro-diffraction patterns one may observe the diffusion unfocused reflexes from the ejected face-centered cubic phase, being expanded from body-centered cubic matrix reflexes in directions, where they should be located at the realization between extractions and the matrix simultaneously for different variants of Kurdyumov–Sachs orientation relation.

Loss of the coherence between copper particles and the matrix, i.e., relaxation of internal stresses as well, as opening of the polygon shaping of the packet martensite, causes the decrease in durability. The heterogeneous character of degradation of the martensite is related to the different velocity of the reactive diffusion in defect free crystals, at their dislocations and at the borders of the crystals.

HIGH PERFORMANCE PLANAR MAGNETRON SPRAYING APPARATUS WITH ROTATING MAGNETIC FIELD

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The proposed innovation relates to an electronic engineering and can be used to produce thin films of materials with improved physical properties using technology of magnetron sputtering in vacuum. It can be used in microelectronics, optics, quantum optics, integrated optics, and nanoelectronics. Magnetron sputtering method with a flat cathode has a significant drawback: on the surface of the flat circular sputtering target electric and magnetic fields are distributedin homogeneously, respectively, on the target surface discharge current densityis non-uniform too. This causes non-uniform wear and, consequently, inefficient (less than 30 %) use of expensive target material. To eliminate this drawback, we have developed an original design of a planar magnetron sputter device with rotating magnetic field. On the basis of this development we have received two invention diplomas (USSR Inventions # 1160761 (1983) and #1244960 (1984)) and one patent (USSR Patent # 1816288 (1990)). We have developed an original design of a rotating magnetic system which provides uniform distribution of discharge current density almost the entire surface of the circle target and, consequently, the formation of a homogeneous area of erosion on the surface. As a result, the target wear is uniform and efficient use of the target material increases significantly (in manufacturing condition up to 70 % and in laboratory conditions up to 90 %) besides ensures high stability and homogeneity of thin film technology. The design is compact and easy to install in any vacuum system. Based on the developed design, we have created a magnetron-sputtering device for laboratory and production of thin films. The use of these devices in production of integrated circuits has greatly reduced manufacturing costs mainly due to saving super clean materials (such as Al, Pt, TiW) and increased device productivity and product quality. We continue to develop the design of planar magnetron sputtering device with a rotating magnetic field. In the magnetic unit we arranged permanent magnets on both sides along specific closed curve obtained by using the original mathematical calculation method. On one side of the curve the magnets have the same poles, and on the other – opposite poles. By variation the distance between opposing magnets we can regulate the magnetic field configuration and the discharge current density, but the shape of the closed curve provides uniform distribution of the discharge current density and, accordingly, all erosion zones on the circle target surface during rotation of the magnetic unit. Simultaneous and individual regulation of the discharge current density and frequency of rotation of the magnetic unit enable to control the spraying process and expand operating facilities in the planar magnetron sputtering device and thus significantly increase the degree of control processes for production of single and multicomponent and multilayer thin films with improved physical properties. On the basis on the results of the study, we obtained two patents of Georgia (GE P 2013 5725 B 2013 01 10, GE P 2016 6512 B 2016 07 11), and the international patent WIPO PCT / GE2016 / 000005, April 26, 2016. As we know, today in research laboratories and manufactures analogous manufacturing apparatus for producing thin films do not have such a high target utilization ratio as our device (70 – 90 %), and the ability of uniform distribution and control the discharge current density is not considered. despite some success in this sphere, to meet new requirements of modern difficult technologies necessary to examine in more detail the processes in a planar magnetron-sputtering device with a rotating magnetic field. Presented here features and innovations (more detailed description of which is not included in this short abstract because of the requirements of protection of copyrights) high-performance planar magnetron sputter coater with a rotating magnetic field show that the developed device may be competitive and interest of professionals.

NEW CHEMICAL METHODS TO FORM METALLIC NANOPARTICLES ON SEMICONDUCTOR SURFACE

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Metallic nanoparticles are the subject of high fundamental and application interests. If the particle sizes are much less then the wave length of excitation light, the particles can posses localized surface plasmons. Such plasmons present collective oscillations of free electrons populated at the metal nanoparticle surface. Excitation of surface plasmons leads to generation of the local electric field in the vicinity of the particles, just providing a wide variety of the plasmon - enhanced optical effects. The latter effects seem to be very prospective for applications in electronic, photonic, photovoltaic devices [1, 2]. For this reason, a search for new well controlled methods to form metallic nanoparticles on semiconductor surfaces is topical. Metalllic nanoparticles are usually formed on semiconductor surfaces by metal vapor deposition with further annealing [3]. We developed an alternative electrochemical method which allows forming on A^3B^5 semiconductor surfaces of the nanoparticles consisting of A^3 metal atoms of the semiconductor [4]. This procedure was used to prepare an array of In nanoparticles on InAs or InP (100) surfaces. For the former case the nanoparticles are formed on InAs (001) surface in electrochemical cell under treating by low-acid (pH ~ 5) water solution of NH_4Cl. When a negative cathode bias is applied to the crystal, hydrated protons H_3O^+ from the solution are reduced to atomic hydrogen H* on the surface. The major part of the reduced H* atoms very readily recombine with formation of molecular hydrogen. Minor part of these H* atoms reacts with InAs at the solid / liquid interface as follows: $InAs + 3H^* = In + AsH_3 \uparrow$.

As a result, In adatoms release and migrate over the crystal surface to form nanoclusters (nanoparticles). Sizes of the formed In nanoparticles depend on treatment duration and the current density. In all our experiments the current density of 20 mA / cm^2 was fixed, and the treatment duration was varied in the interval of 12 – 18 min. Under these conditions, nanoparticle sizes occur to be in the interval of 30 – 60 nm. The In nanoparticle arrays formed on InAs (100) surface were studied by scanning electron microscopy (SEM) and atomic force microscopy (AFM). The both diagnostic techniques reveal In nanoparticles of nearly uniform sizes randomly distributed on the surface. Shape of In nanoclusters as seen from SEM image is ellipsoid-like with slight oblateness along the normal to InAs surface. Similar In clusters were observed to form on InP (100) surface after electrochemical treatment.

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MAGNETITE / SILICA NANOCOMPOSITES AS SOLID-PHASE EXTRACTANTS FOR HEAVY METAL IONS

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Heavy metals are widely known among the major environment pollutants. They are especially dangerous for hydrobionts. Currently, hardly any surface water reservoir in Ukraine can be attributed to the first category (with water is suitable for drinking), according to the degree of water pollution, environmental and basic sanitation conditions, chemical and microbiological parameters. Therefore, effective extraction of heavy metal ions from wastewater and water reservoirs is an up-to-date problem nowadays. Magnetite nanoparticles functionalized via sol–gel method using alkoxysilanes have become common object of study [1, 2]. They can be used in different areas of science, such as biotechnology [3, 4] or target drug delivery. In addition, they are prospective adsorbents through their magnetic sensitivity (comparing with silica-based samples) [5, 6]. Generally, the properties of such materials (size of the particles, specific surface hydrophilicity of the surface, functional groups) depend on alkoxysilanes used as precursors.

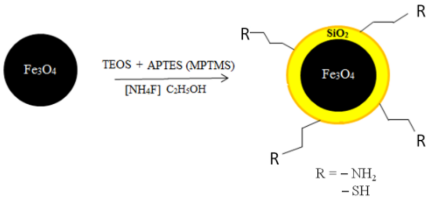

Figure 1. Using sol–gel method for magnetite functionalization.

In this work we were focused on synthetic procedures of mono- and bifunctional nanocomposites production (the general scheme is presented in the **Figure 1**) as the continuation of the previously started research [7]. Afterwards, the adsorption properties of the synthesized materials in relation to the heavy metals (Ag^+, Hg^{2+}, Pb^{2+}, Cd^{2+}) were investigated and compared.

The current research was financed by NASU–NASB Joint Project (06–03–15) and the SASPRO Program No. 1298 / 03 / 01.

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ON THE INFLUENCE OF THE TEMPERATURE ON Ag NANOPARTICLES WATER DISERTIONS IN POLYMER MATRIX FORMING

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The most extensively investigated route for developing silver nanoparticles (Ag NPs) is chemical method where silver salt in polymer matrix solution is reduced by reducing agents. The nature and structure of the polymer matrices affect the shape and size of the particles. Obviously, the internal structure of macromolecules should affect the process of nanoparticle formation.

The present study is scoped on silver nanoparticle *in situ* generation using branched and linear polyacrylamide matrices. The branched polymer structures demonstrate an improvement of ordering phenomenon, so such systems can differ in functionalities from their linear analogues.

The formation of Ag NPs was observed by the appearance of brownish-red solution color and intensive surface plasmon absorption band in the range of 390 – 410 nm. The influence of the internal structure of the host polymer and the temperature on the Ag NPs generation, their size distribution were studied by UV–Vis spectroscopy (**Figure 1**), dynamic light scattering (DLS) and transmission electronic microscopy (TEM).

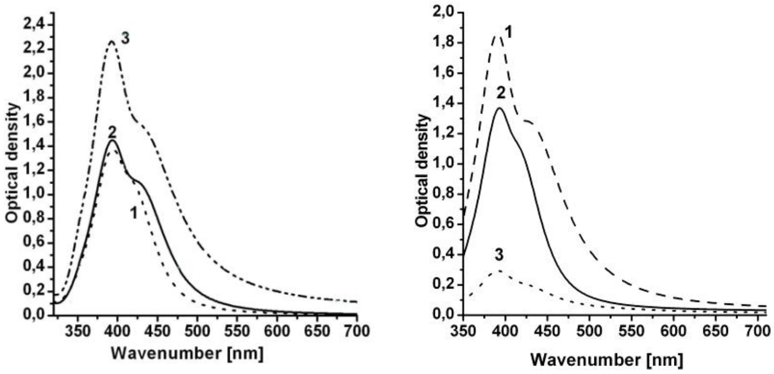

Figure 1. UV–Vis spectra of Ag NPs synthesized in D-g-PAA (on the left) and linear PAA (on the right) matrix at 20 (1), 40 (2) and 80°C (3).

Stable silver colloids were obtained in temperature range of 0 – 80 °C in nonionic and anionic D-g-PAA matrices. For nanosystems synthesized at 80 °C in linear nonionic PAA matrix active oxidation and aggregation process have been observed. Silver colloids fabricated in the anionic linear PAA matrix were unstable even at the room temperature, while in star-like D-g-PAA anionic host polymer the colloids were stable for a long time after. Analysis of to DLS and TEM data revealed the average size of Ag NPs of 5 – 20 nm. Size distribution functions for all simples had the binodal character with maximums located in the range of 5 – 8 and 12 – 16 nm and were depended on the type of polymer matrix and the synthesis conditions.

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LOW-TEMPERATURE METHOD OF FORMATION OF GROUP III NITRIDE (GaN, AlN) NANOFILMS

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Group III nitride (GaN, AlN) as an electronics material attracts great interest of scientists and researchers. Devices based thereon have a number of unique features: high gain, light emission in a wide spectral range, stable performance at high temperatures and radiation, and the possibility of making wideband wireless circuits, compact and reliable radars for aircraft and space applications, which makes them even more promising [1].

Preparation of nitrides in the crystalline forms is difficult due to high melting temperatures. The formation of nitrides is performed at high temperatures and pressures. However, the resulting structures are amorphous, and to produce polycrystals, the subsequent high-temperature (above 1000 °C) processing is required. This complicates the introduction of the material in production. Therefore, their preparation in the form of films is more preferable [2]. Thin films are nanosystems in which nano-sizes occur only in one direction - in thickness, and the other two directions are micro-sized.

There are various methods of obtaining nanofilms: molecular beam or liquid epitaxy, chemical vapor deposition (CVD), extraction from colloidal solutions and deposition, Langmuir-Blodgett technology, metal-organic chemical vapor deposition (MOCVD), etc. [3]. However, all these methods are generally high-temperature, and at relatively low temperatures the process proceeds too slowly. Therefore, it is desirable to find a technological method that will eliminate completely, or at least partially, the above mentioned disadvantages.

In the work, the possibility of formation of GaN and AlNnanofilms at relatively low temperatures (300 – 700 °C) by magnetron sputtering of gallium and aluminum in the nitrogen atmosphere, under ultraviolet light, followed by a pulsed photon annealing is reported. It is shown that the pulse photon annealing forms polycrystalline inclusions in the initially amorphous gallium nitride and aluminum nitride.

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NANOSCALE HfO_2 AND ZrO_2 GATE OXIDES IN FIELD EFFECT TRANSISTORS

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Nanoscale HfO_2 and ZrO_2 oxides have been received by low temperature technology – plasma anodizing with ultra violet stimulation and based on fabricated field effect transistor (FET) [1]. Oxidation process carries out at relatively low temperature (400 °C) and distinguished as a clean, vacuum and easy process. In the first stage of experiments were used hafnium (Hf) and zirconium (Zr) as a metals deposited onto silicon substrate and following oxidation by plasma anodizing to investigate there electric properties and then use them in the single-gate and dual-gate [2 – 4] transistors as a gate dielectrics. The properties of received oxides and transistors were characterized $I - V$ and $C - V$ measurements, XPS spectrometer and SEM measurements.

Creation integrated circuits elements include several key technological processes and the one of them is formation dielectric films. Dielectric is a main component for the integrated circuit, which is responsible for the electrical isolation of the circuit elements, the active element in the field effect transistors as a gate dielectric and generally in the metal–oxide–semiconductor (MOS) structures.

Formation of dielectric films in the world happens at high temperatures (1100 °C). At this temperatures take place diffusion of unwanted impurities, increasing porosity, becoming worst adhesion to the substrate and etc. [5]. All of this influences badly on the parameters of nano-scale devices. Progress in the development of nanotechnologies the high temperature became unsupportive process, because reducing the size of the nanostructures it changes physical and chemical properties of the material.

Hafnium and Zirconium based oxides replacesilicon dioxide as a gate insulator in field-effect-transistors. The advantage for transistors is its high dielectric constant: the dielectric constant of HfO_2 and ZrO_2 is 4 – 6 times higher than that of SiO_2 [6, 7].

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QUANTUM DOTS: GENESIS, THE EXCITONIC ZOO, AND NANO-PHOTONICS

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Universal self-organization and self-ordering effects at surfaces of semiconductors lead to the formation of coherent zero-dimensional nanoclusters called quantum dots (QDs). The electronic and optical properties of QDs, being smaller than the de-Broglie-wavelength in all three directions of space, are closer to those of atoms in a dielectric cage, than of solids. Their delta-function-like energy eigenstates are only twofold (spin) degenerate. All few particle excitonic states are strongly Coulomb correlated. Their energies depend on shape and size of the dots, such that positive or negative biexciton binding energies or fine-structure splitting caused by exchange interaction appear.

Consequently, single QDs present the most practical possible basis of emitters of single polarized photons (Q-bit emitters) on demand or entangled photons via the biexciton–exciton cascade for future quantum cryptography and communication systems.

Semiconductor nanotechnologies transform presently to enabling technologies for new economies. It is expected that first commercialization of nanophotonic devices and systems will appear soon. High bit rate and secure quantum cryptographic systems, nano-flash memories, or ultra-high speed nanophotonic devices for future optical interconnects, the Terabus, and 100 – 400 Gbit / s Ethernet might present some of the first fields of applications of nanophotonic devices.

SYMMETRY ASPECTS OF OPTICAL ACTIVITY FOR $Hg_3Te_2Br_2$ CRYSTALS

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$Hg_3Te_2Br_2$ crystals, one of the ternary chalcogenide-halogenides materials, belong to the $Hg_3X_2Y_2$ (X = S, Se, Te; Y = F, Cl, Br, I) family of compounds with corderoite structure. An acentricity of the crystal structure of mentioned crystals is one of the reasons to forecast their possible application also as non-linear optical material. It should be noted that they are described by the $T^5 – I2_13$ space symmetry group that confirmed a presence of optical activity and electro-optic effect for these crystals [1 – 3], which make them perspective nanomaterials for nonlinear optics and optoelectronics.

According to a theory of optical activity, thenature of light wave polarization in an optically active crystal include normal component of gyration tensor in ***k*** vector direction. Itisfullydeterminedby symmetry of G part and gyration tensor consider asa symmetrical. The pointing surface symmetry of gyration tensor for body-centered cubic crystals $T^5 – 2_13$ describes by the ∞∞ symmetry class of optical activity. The eigenvalues of gyration tensor are: $g_{11} = g_{22} = g_{33} = g$ and non-diagonal elements are zero for this case [1]. The gyration tensor for $Hg_3Te_2Br_2$crystals is calculated.Temperature dependence analysis ρ (T) for $Hg_3Te_2Br_2$ crystals shows that displacements of absorption edge are played the main role, because the optical rotation power is not depended on temperature. The direct interband transitions in $Hg_3Te_2Br_2$crystals are localized on [$HgTe_2Br_4$] structural complexes. The deformation degree of these complexes caused by internal crystal field will determine the strength of transition rotation and optical activity value of crystals. Optical activity of $Hg_3Te_2Br_2$ crystals has molecular origin and associated with induced asymmetrization of [$HgTe_2Br_4$] chromophore, which is determined by space symmetry group of these crystals.

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THEORETICAL ANALYSIS OF OPTICAL PROPERTIES FOR Tl_3XY_4 CRYSTALS

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The present paper is aimed at the theoretical studies of refractive indices and reflection coefficients forTl_3XY_4 (X = V, Nb, Ta; Y = S, Se) crystals. The structure and its couplings to the fundamental physical properties of thesecompounds is very interesting subject for theoretical studies due to their foreseen practical usage possibilities. The main feature of ternary thallium chalcogenides is formation of numerous polymorphic modifications and existence of isomorphic substitations in sublattices. Interest in them is caused by the ability to form continuous raw of solid solutions that allows use them for different variations of physical and chemical properties. The specific feature of mentioned structures is the presence of [XY_4] and [TlY_8] structural complexes. Due to their unique physical and chemical properties these crystals in nanoparticle form have a wide range of applications in non-linear optics.

It should be noted that the refractive index is one of fundamental properties of a material because it is closely related to the electronic polarizability of ions and the local field inside the material. Besides that theoretical study of refractive index gives more detailed information about crystals properties.Origin of the chemical bonding in crystals is very important for definition of the physical and chemical properties. The refractive index evaluation is of considerable importance for applications in integrated optic devices, where materials refractive index is the key parameter for device design. Optical properties for Tl_3XY_4 crystals are calculated according to the model proposed by Harrison [1 – 3]. The refractive index in the spectral region far from the absorption edge is determined within the generalized single-oscillator model. It follows from the theoretical considerations that the Harrison's approach is a convenient and flexible approach for the study of optical properties.

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THE IMPACT OF VACANCY DEFECTS ON THE ELECTRONIC STRUCTURE OF $Hg_3Te_2Cl_2$ CRYSTALS

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$Hg_3X_2Y_2$compounds are crystallized into corderoite structure. The structure and its couplings to the fundamental physical properties of these compounds is very interesting subject for theoretical studies due to their foreseen practical usage possibilities. The main structural feature of $Hg_3X_2Y_2$ mercury chalcogen halogenides is the tendency to formation of various polymorphic modifications [1 – 3]. Additionally, in this class of the materials point defects of lattice structure are the significant contributors to their applications.

In this paper, the DFT calculations are used to investigate the impact of point defects on electronic structure of $Hg_3Te_2Cl_2$ crystals by using the supercell model [2 × 2 × 1]. The *ab initio* calculations for defect-free and defective $Hg_3Te_2Cl_2$ crystals in the LDA approximation using the quantum-chemical software package SIESTA are performed for the first time. The studied crystal possesses an indirect band gap. According to the analysis of the obtained data, the indirect gap is 2.628 eV while the direct gap is 2.714 eV. Satisfactory agreement is obtained with the experimental data. Influence of vacancy defects on conductive and optical properties of $Hg_3Te_2Cl_2$ crystals is discussed in details. It is established that all additional levels are formed due to the cation and anions hybridization. The anion vacancies modify energy band structure that reflects on the electronic and optical properties of the $Hg_3Te_2Cl_2$ crystals. It is found that the presence of point defects in $Hg_3Te_2Cl_2$change the direction of optical transitions and therefore the defective crystal is direct gap semiconductor. The electron density maps demonstrate presence of covalent Hg=Te and ionic Hg=Cl bond character. In addition, anion vacancies influence greatly the geometry structure of the surrounding atoms, and the great relaxation of surface occur, which results in the alteration of the electronic properties for $Hg_3Te_2Cl_2$ crystals.

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DEGRADATION OF THE ORGANIC COMPOUNDS BY SILVER NANOPARTICLES UNDER LOCAL PLASMON RESONANCE CONDITIONS

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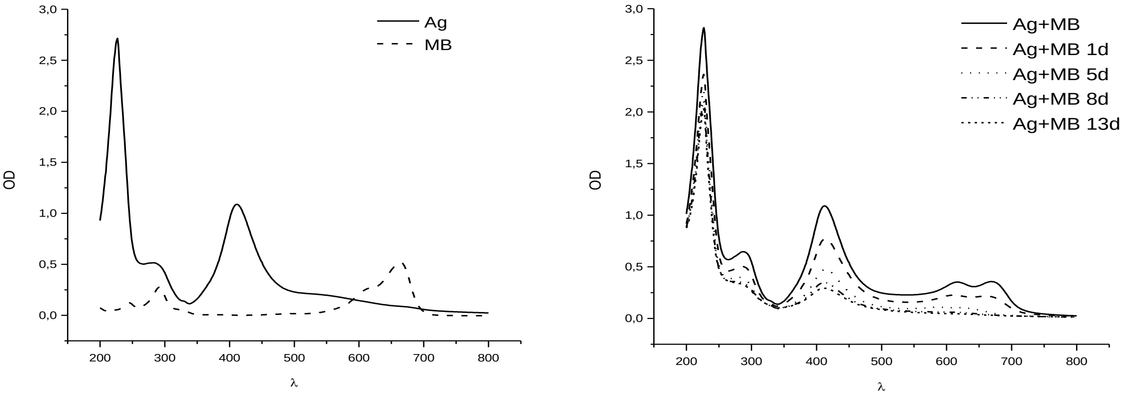
The approach based on the idea of conducting chemical reactions under the conditions of surface plasmon resonance is quite promising with regard to the controllable selective degradation of certain organic substances, which could be applied, for example, for the control of the water quality etc. Because of characteristic features of the light field distribution in direct proximity to the metal surface the local intensities of surface electric fields can reach high values. In this case it is possible to lower or completely level out the potential or activation barriers, giving rise to the occurrence of reactions that are impossible under normal conditions.

Silver nanoparticles (Ag–NP) are known to have oxidizing properties with respect to organic substances and have found use, for example, as oxidant for exhaust gases generated during operation of automobile engines. Aqueous solutions of colloidal Ag–NP also possess oxidative properties with respect to organic compounds under the action of light radiation. The most convenient way to study oxidative properties of colloidal silver solutions is the use as test reactions of certain organic dyes, for example, methylene blue. Methylene blue is a typical representative of heterocyclic organic compounds and can serve as a convenient indicator to measure.



a b

Figure 1. (a) Spectra of Ag–NP and methylene blue;
(b) Decomposition of methylene blue by Ag–NP in time.

The aim of this work was to demonstrate the possibility of the controllable degradation of organic compounds by Ag-NP under local plasmon resonance conditions on the example of methylene blue. Ag-NP and methylene blue have well distinguishable peaks of absorption (**Figure 1a**), which make the action of Ag-NP on methylene blue clearly evident. Decomposition of methylene blue demonstrated on the **Figure 1b** is a result of oxidation on silver nanoparticles when exposed to visible light. As a result of exposure to visible light under local plasmon resonance conditions "dangling bonds" were formed on the surface of the nanoparticles, which include free electrons and free valencies. In this process, the active form of silver ions interact with methylene blue to form complex compounds. Further interaction with silver nanoparticles subsequently converted to products of the decomposition of organic matter until elementary compounds. Thus as a result of chemical reactions taking place the destruction of consumed silver nanoparticles.

FORMATION AND GROWTH OF GOLD NANOSTRUCTURES ON ATOMICALLY SMOOTH SURFACES OF MoS_2, GRAPHITE, MICA IN THE NON-AQUEOUS MEDIUM

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The gold nanoparticles (NPs) is widely used in different applications due to their unique optical and catalytic properties. Physical properties of such NPs strongly depend on their shape and size which can be controlled by tuning of synthesis conditions. A numerous methods of synthesis of NPs allow obtaining spherical and anisotropic Au NPs in aqueous and non-aqueous media, in the micelles and at the phase interfaces. For following characterization nanoparticles are being delivered to the surface of various materials. We propose to grow the Au NPs directly on atomically flat surfaces of different monocrystals: MoS_2, highly oriented pyrolytic graphite (HOPG) and mica.

It has previously been shown [1] that flat triangular and hexagonal gold nanocrystals with a thickness less than 100 nm can be formed in free volume of mixture of ethanol (ET), ethylene glycol (EG), $HAuCl_4$ (a precursor of gold) and stabilizer polyvinyl pyrrolidone (PVP) at 80 °C. Immersing to the growth medium [1] the plates of freshly cleaved MoS_2, HOPG or mica drastically changes the synthesis conditions and leads to a qualitative and quantitative difference between nanostructures obtained in free volume and on the surfaces. Thus, the spherical NPs and monocrystals are being formed preferentially in presence of the mica and graphite surfaces, while on MoS_2–NPs and Au nanowires.

We have changed the conditions of synthesis by adding the glycerin in growth medium. Thereby the viscosity of the dispersion medium and the wetting ability of substrate surface were increased. It was found that the gold NPs have been formed on all immersed substrates at a volume ratio of EG–ET–GL (7 : 7 : 6) and at concentrations of C_{Au} = 1 mM, C_{PVP} = 0.045 M at 80 °C during 5 h. Nanoprisms were mainly formed on the mica surface after 48 h, on MoS_2 – nanowires, nanoprisms and NPs, on graphite – nanoprisms and NPs with more complicate shape. Such difference in formation of nanostructures on the atomically smooth surfaces of MoS_2, graphite and mica is related to the nature of the immersed surface, mobility of gold atoms.

The shape, size and thickness of the gold NPs were estimated by scanning electron microscopy. The method of electron microprobe analysis has revealed that the gold NPs have no incidental impurities. It has been found that the distribution of gold NP is accidental on the mica surface, while the formation of nanowires on MoS_2 surface was observed preferentially close to defects, which are most likely associated to sulfur atoms on the surface. The conditions of synthesis and formation of gold nanostructures on the atomically smooth surfaces of MoS_2, graphite and mica have been established. Obtained nanostructures can be used in micro- and nanoelectronics, sensing, catalysis.

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MANGANIUM OXIDE DOPING INFLUENCE ON THE STRUCTURE OF HYDROXYAPATITE LAYER BUILD ON THE Na_2O–CaO–B_2O_3–SiO_2–P_2O_5 GLASS SURFACES

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Silicon–phosphorous glasses are focusing a wide attention due to their bioactivity, being a good base for hydroxyapatite layers growing. Recently, it was discovered that small addition of transition metal ions may enhance bio-properties of the material [1, 2].Here we report structural features both of a Na_2O–CaO–B_2O_3–SiO_2–P_2O_5 glass doped with different amounts of Mn ions and hydroxyapatite layer grown during an immersing of glass samples in simulated body fluid (SBF). Results of DSC, XRD, Raman (**Figure 1**), SEM (**Figures 2** and **3**), and AFM measurements will be presented and discussed in the context of the Mn ions influence. Surface modifications generated by a presence of Mn ions strongly change behaviour of the samples during a immersing in SBF. It occurs that the structure of the apatite layer, specially dimensions of apatite nanograins, depends on the amount of doping ions in the glass.

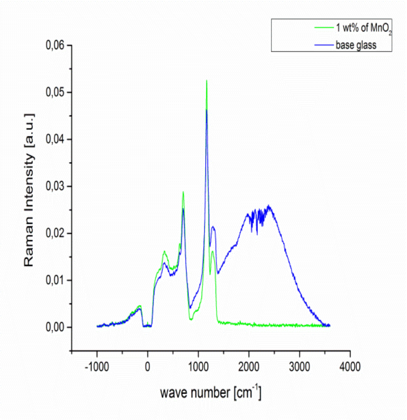

Figure 1. Raman spectra: base glass – green, glass with 1 wt. % of MnO_2 – blue.

Figure 2. SEMimage of base glass surface.

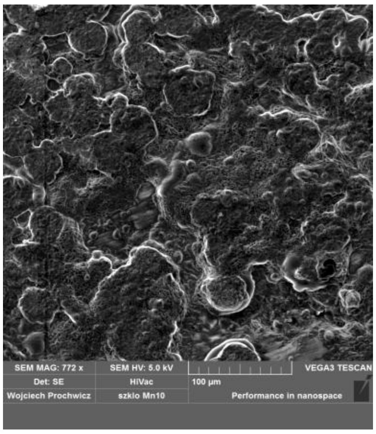

Figure 3. SEM picture of glass with 1 wt. % of MnO_2.

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LASER-INDUCED NANO-SCALE FLUORENCE RESONANCE ENERGY TRANSFER IN DNA

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The nano-scale method of laser-induced fluorescence resonance energy transfer (FRET) to donor-acceptor intercalator pair for quantitative and qualitative study of stability quality, the DNA double helix in solution in real time is offered. The approach is based on the example of the acridine orange molecule (donor) and ethidium bromide (acceptor) intercalated in DNA [1].

It is shown that ions Cu(II), Cu(I), Ag(I), and AgNPs, laser irradiation of AO, and the effect of heating decrease the concentration of undamaged areas of DNA double helix, i.e., the sites able to intercalate dye molecules such as AO and EB.

FRET radii were experimentally estimated in the background electrolyte solution (0.01 mol / l $NaNO_3$) and proved to be 3.75 ± 0.3 nm, and the data are in satisfactory agreement with the theoretically calculated value R_0 = 3.71 ± 0.3 nm (AO quantum yield q_{0D} = 0.75, refractive index n = 1.4 and orientation factor $k^2 = (2/3) \times 0.84$).

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ADSORPTION AND SORPTION CHARACTERISTICS OF ORGANIC MATERIALS IN METAL ION REDUCTION REACTION AND NANOTECHNOLOGY

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Our aim is to apply adsorption and sorption characteristics of DNA, PAMAM – dendrimere, cellophane membranes, human hair and cotton fibber in copper and silver ion reduction to atomic state. Based on DNA – silver complex interactions of structures having identical chromophore and hard structure are demonstrated widening of DNA–silver absorption spectra (**Figure 1**). Interactions of silver ions with DNA are characterized by inter- – cross-type of links which reduce dynamic properties of double helix and make it harder.

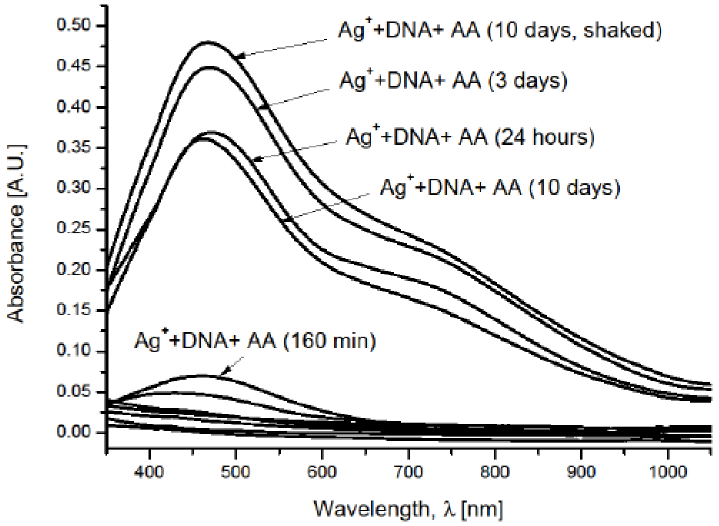

Figure 1. Spectra for silver ion reduction (AA – ascorbic acid) in complexes DNA–$AgNO_3$–AA. [DNA] – $5.9 \cdot 10^{-4}$ M(P), [$AgNO_3$] – $1.2 \cdot 10^{-4}$ M, [AA] – $2.4 \cdot 10^{-4}$ M, [$NaNO_3$] – $1.0 \cdot 10^{-2}$ M.

The reason for spectrum widening is further condensation of reduced silver ions in clusters and nanoparticles with the size of more than 50 nm.

EFFECTS OF FUNCTIONAL ADDITIVES ON THE SELF PROPAGATING HIGH TEMPERATURE SYNTHESIS (SHS) OF NANO ZrB_2 AND B_4C POWDERS

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There are many production methods for the synthesis of boride based advanced nano ceramics such as carbothermic reduction, synthesis from elements, gas phase reactions and self-propagating high-temperature synthesis (SHS). Self-propagating high-temperature synthesis is one of the important methods to synthesize advanced materials such as ceramics (e.g. ZrB_2, TiB_2, B_4C, Si_3N_4); abrasives, cutting tools and polishing powders (e.g. TiC, cemented carbides); resistive heating elements (e.g. $MoSi_2$), shape-memory alloys (e.g. TiNi); high-temperature structural alloys (e.g. nickel aluminides); master alloys (e.g. AlTiB); neutron attenuators (e.g. refractory metal hydrides) as well as conventional metals and their alloys[1,2].

The advanced thermochemical simulations of the reactions were investigated in detail including different ratios of initial mixtures, as well as different initial temperatures in order to reduce the number of experiments. In addition, the adiabatic temperatures were calculated for each system by using FactSage 6.2 Termochemistry simulation software.

In the experiments firstly ZrB_2 and B_4C production parameters were investigated. Some stoichiometric mixtures were prepared and SHS experiments were carried out. The obtained SHS products were discharged and milled below 45 μm and then leached with aqueous of the stoichiometric HCl (80 °C, 60 min, 400 rpm, 1 / 20 solid / liquid ratio). Leach cakes were dried and characterized. The optimum SHS conditions were determined, these were molar ratio [B_2O_3 : Mg : C (1 : 3 : 0.8)] for B_4C and [ZrO : Mg : B_2O_3 (1 : 3 : 6)] for ZrB_2.

In the second experimental set effect of functional additives were investigated to improve efficiency and surface area of products. In B_4C synthesis experiments $KClO_3$, $KHSO_4$, $MgSO_4 \cdot 7H2O$, NaCl, MgO and Na_2SO_4 added to the selected mixture and their effects were examined. In ZrB_2 production experiments, KCl_4 and NaCl supplement to the chosen mixture and their effects were investigated. The XRD analysis showed that main phases of the SHS product were MgO and ZrB_2. After the SHS process, ZrB_2 was separated from byproducts MgO, $Mg_3B_2O_6$ and $Mg_2B_2O_5$ by HCl acid leaching. KCL_4 and NaCl additives effected negatively to leach parameter $Mg_3B_2O_6$ and MgB_4O_7 phases could not be removed on 1.88 M HCl solution at 1 / 20 S / L ratio for 60 min at 80 °C leach conditions. On the other hand BET analyses revealed that the products has higher surface area with KCL_4 and NaCl additives. Similar effects detected in B_4C experiments and surface area increased from 15.4 m^2 / g to 30 m^2 / g.

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ZnO-PHTHALOCYANINES HYBRID NANOSTRUCTURED FILMS AS SENSITIVE LAYERS FOR CHEMICAL SENSORS ARRAYS

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Hybrid organic-inorganic nanostructured layers are of significant interest for the development of sensitive layers for chemical sensors and arrays. Nanostructured surface usually allows to increase the sensitivity and stability of sensor response comparing with “flat” film of the same material. This is due to the increase of the surface area. But in the same time, the combination of certain semiconducting materials opens wide possibilities for the directed control of the adsorption properties of the resulted hybrid film.

We investigated the adsorption properties of the composites made of ZnO nanostructured under layer and a 30 nm phthalocyanine (Pc) thermally sputtered on it. There were two types of ZnO layers obtained from the same solution of dodecylamine-stablized ZnO NP: (1) dropped from the solution with following drying under room temperature (DP) and (2) pulverized on the heated (150 °C) quartz crystal microbalance (QCM) sensor’s surface (PV) [1]. The Pcs (metal free Pc – H_2Pc; copper Pc – CuPc; lead Pc – PbPc) were thermally sputtered on the nanostructured under layer.

The two types of ZnO under layer have different surface structures (seen form TEM images, [2]) and different adsorption properties. The DP one is highly developed porous surface while the PV layer has two phases: amorphous organic one and ZnO NP aggregates. DP ZnO layer demonstrates linear dependences of QCM response to different alcohols. The PV film demonstrates higher sensitivity and has linear dependences at low concentrations but the response starts to decrease starting from certain analyte concentration, supposedly, due to swelling of the film.

The two types of ZnO layers are of interest for creating of chemical sensors due to their high sensitivity and variability of the response to different analytes. The adsorption properties of H_2Pc, CuPc and PbPc were previousely investigated in [3]. Interaction between donor Pc and acceptor ZnO affects the adsorption centers of the Pc film. The combination with ZnO nanostructured layers increases the sensitivity of Pc films (about one order at low concentrations) but, what is more important, changes their adsorption behavior as well. The combination of Pcs with ZnO NP opens wide field for the creation of chemical sensors with overlapping but different sensitivity profiles – exactly what is necessary for cross-reactive sensor arrays for electronic nose technology.

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NMR TECHNOLOGY FOR DETECTION OF AMMONIUM NITRATE AND DERIVATIVES

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Ammonium nitrate (NH_4NO_3) is agricultural fertilizer, which is produced in industrial quantities in Georgia. AN belongs to dual use chemical, as is potent explosive and detonator. There are risks associated with the use of AN. In airbags is used ammonium nitrate-based propellant. 2014 were announced about recall of cars with airbags manufactured by TAKADA with the defect that improperly inflate the airbags. There have been 10 deaths and more than 100 injuries due to this problem in the U.S. On 22 July 2011, in the Oslo bombing explosion was used AN explosive (ANFO) before the building housing the Office of the Prime Minister and Ministry of Justice and the Police. In several European Countries is banned use of AN, e.g. Germany and Ireland. In 2008 Ammonium Nitrate Security Program was proposed by the USA Department of Homeland Security (DHS) in response to direction from Congress to "regulate the sale and transfer to prevent the misappropriation or use of ammonium nitrate in an act of terrorism" [1]. The fertilizer is banned in Afghanistan because it's an easy ingredient for Home Made Explosives (HME) in 2010.

In US Sanida National Laboratories in 2013 by Kevin Fleming was developed formula, which was not patented. Invention is the combination of iron sulfate with ammonium nitrate and resulted in an effective and cheap fertilizer which is useless as a component in an ANFO explosive; iron sulfate becomes iron nitrate and ammonium nitrate becomes ammonium sulfate. This metathesis reaction occurs if someone tries to alter the fertilizer to make it detonatable when mixed with a fuel [2].

In our study we are applying innovative method of NMR spectroscopy for the fast and reliable detection of nitrogen containing compounds. With this technique is possible to study composition of synthesized compound at all stages of chemical synthesis, as well to test final product.

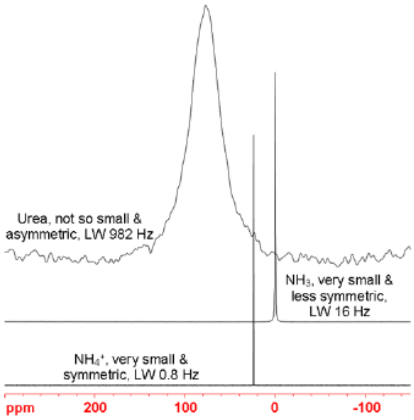

Figure 1. ^{14}N NMR signals of NH_4^+ and NH_3. Comparison of line-widths of ^{14}N signals. The larger and less symmetric the molecule, the wider the signal.

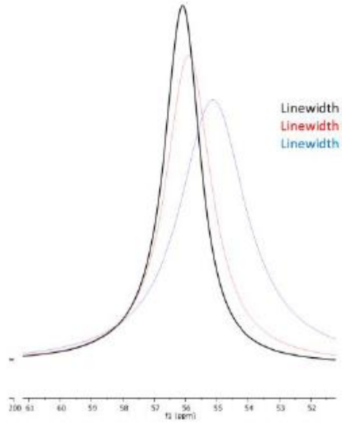

Figure 2. Line widening is observed when other molecule is interacting with NH_4^+ non covalently (right. Authors' own results). Left image used with permission [1].

Here we consider scientific confirmation for safety applications of NH_4NO_3, for threats and consequences management of ammonium nitrate. Fertilizer it's a mix of $(NH_4)_2SO_4$, the double salts $(NH_4)_2SO_4{\cdot}2(NH_4NO_3)$ and $(NH_4)_2SO_4{\cdot}3(NH_4NO_3)$, and a trace of NH_4NO_3. Agronomic tests show that the material works just as well as conventional ammonium nitrate or ammonium sulfate fertilizers (**Figure 1**).

While ammonium molecule provides sharp peaks on spectrum, when ion is attached to larger molecule we observe broadening of the line-width, which is demonstrative for ammonium bound to other molecule (**Figure 2**).

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SYNTHESIS OF ENERGETIC COMPOSITES IN Ti–Al–B–C SYSTEM

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Recent developments in materials science have increased the interest towards the bulk (energetic / energy) materials and the technologies for their production. The unique properties which are typical for the composites fabricated in Ti–Al–B–C systems makes them very attractive for aerospace, power engineering, machine and chemical applications. In addition, aluminum matrix composites (AMCs) have great potential as structural materials due to their excellent physical, mechanical and tribological properties. Because of good combinations of thermal conductivity and dimensional stability AMCs are found to be also potential materials for electronic packaging/application. The methodology and technology for the fabrication of bulk materials from ultrafine grained powders of Ti–Al–B–C system are described in this paper. It includes results of theoretical and experimental investigation for selection of powder compositions and determination of thermodynamic conditions for blend preparation, as well as optimal technological parameters for mechanical alloying and adiabatic compaction. The crystalline coarse Ti, Al, C powders and amorphous B were used as precursors, and blends with different compositions of Ti–Al, Ti–Al–C, Ti–B–C and Ti–Al–B were prepared. Preliminary determinations / selections of blend compositions were made on the basis of phase diagrams. The powders were mixed according the selected ratios of components to produce the blend. Blends were then processed in high energetic planetary ball mills for mechanical alloying, syntheses of new phases, amorphization and production of nano and ultrafine powders. The blends processing time ranged from 1 to 24 h. The optimal technological regimes of nano blend preparation were determined experimentally. The ball milled nano blends were placed in metallic tubes and loaded by explosive energy for furtherconsolidation and synthesis in adiabatic regime. The effect of the processing parameters on the structure and properties of the nano and ultrafine materials was investigated and is discussed here. For consolidation of the mixturesthe explosive compaction technology was applied at room temperatures. The relationship of the ball milling technological parameters and the consolidation conditions on the structure / properties of these materials is presented and discussed in this paper.

PLANAR CLUSTERS OF IDENTICAL ATOMS IN EQUILIBRIUM: DIATOMIC MODEL APPROACH FOR BORON

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Diatomic model, when is utilized to describe clusters of identical atoms, takes into account bonding only between neighboring pairs of atoms.

Isomers of wrapped forms, e.g. built from nanotubular and / or fullerene-like structural fragments, according to diatomic model have to be more stable energetically than their planar counterparts because planar clusters contain more peripheral atoms with dangling bonds and, correspondingly, lesser atoms with saturated bonds.

At the same time, difference in coordination numbers between central and peripheral atoms in planar clusters leads to the bonds polarity. Introducing corrections related to electrostatic forces reveals that small planar clusters can be more stable than their wrapped isomers.

There is provided a general theoretical frame for studying the planar clusters of identical atoms, which is numerically realized for all-boron planar clusters.

PHOTO-ELECTROCHEMICAL PROPERTIES AND PHOTOCATALYTIC ACTIVITY OF NANOSIZED NITROGEN AND IRON DOPED TiO_2 FILMS

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Widespread use of semiconducting photocatalysts for environmentally important processes of neutralization of toxic organic compounds of and heavy metals in the waste water, drinking water and air is caused by the essentials to create the new nanomaterials with the high surface area, the define structure as well as the enhanced activities under both UV and visible light irradiation, improving the efficiency solar energy utilization. Doping with nonmetals (B, C, N, S or F) or metals (Fe, Cr, Co, Mo or V) have been employed to tune the electronic structure and enhance the photocatalytic activity of titanium dioxide based materials under visible light.

Herein, we report a simple preparation method of nitrogen-doped TiO_2 and Fe/TiO_2 films, their structure, photoelectrochemical characterization and photocatalytic properties under both UV and visible-light in photoreduction of Cr(VI) ions to Cr(III) and degradation of biogenic (antropogenic) pollutant – tetracycline hydrochlorite as a representative class of antibiotics. The photo-electrochemical properties of the TiO_2, Fe / TiO_2 and N / Fe / TiO_2 electrodes were estimated using the spectral dependence of the photocurrency. Energy level diagrams of synthesized films were designed by the direct electrochemical measurements that allowed predicting the activity of the semiconductors in the photocatalytic processes.

The films containing iron ions showed lower photocurrent quantum yield than that for undoped samples. Iron and nitrogen doping leads to the cathodic shift of the conduction band bottom (ΔE_{cb}) along with the band-gap energy (E_g) decrease. The most significant changes of flat band potential values were observed for nitrogen contained Ti : Fe = 1 : 1 samples that probably related to the $Fe_2Ti_2O_7$ phase formation under 450°C heating. Multicomponent N / Fe / TiO_2 films synthesized by sol–gel method and treated at a relatively low temperature (450 °C) contain the pseudobrukite structure (Fe_2TiO_5) with landaunite ($Fe_2Ti_2O_7$) impurities. Nitrogen incorporation in the film structure leads to the accumulation of iron ions on the surface of the material and acceleration of the $Fe_2Ti_2O_7$ phase formation while pseudobrookite particle size is reduced compared with Fe / TiO_2 systems. High photocatalytic activity of the film correlates with its high adsorption capacity.

PHOTO STIMULATED FLUORESCENT ENHANCEMENT AND OPTICALLY CONTROLLED DRUG RELEASE BASED ON GOLD NANOPARTICLE CONJUGATED ORGANIC DYE NANOCOMPOSITE, AND THE SPIROPYRAN DOPED LIQUID CRYSTAL MICROSPHERES

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In this study, we describe light activated fluorescent enhancement and optically controlled drug delivery, based on gold nanoparticles (GNPs) conjugated organic dye nanocomposite (a), and the spiropyran doped liquid crystal microspheres. First platform aims to visualize the cancer cells and the other one (b), to deliver the specific drug molecules in the targeted placement and at the controlled portions.

(a) We present here GNPs formed and incorporated together with luminescent dye Nile blue (NbD) into a Poly (vinyl alcohol) film. The increase of luminescence of the NbD results from its interaction with GNPs surface plasmons. The electric charge on the GNPs and the distance between GNPs and luminescent dye molecules has a significant effect on the luminescence intensity, and this enhancement depends strongly upon the wavelength of the incident light. Enhancement in luminescence using GNPs / NbD complex will lead to many applications for advancement in biomolecular labeling to produce novel optical contrast agents with high sensitivity and specificity. These results may have great importance in chemotherapy, in cancer diagnosis [1].

(b) In this work, we have demonstrated a novel, light controlled drug delivery system, based on spiropyran (SP) doped liquid crystal (LC) micro spheres. Experimental results have shown that upon exposure to UV / Violet light, the photochromic molecules located inside the LC spheres, experience an interconversion from the hydrophobic, oil soluble, non-polar SP state, to the hydrophilic, water soluble, highly polar *merocyanine* (MC) state. Light induced photoisomerization destabilize LC water interface, stimulates the translocation of MC molecules across the LC–water barrier and results their homogeneous distribution throughout in an aqueous environment [2].

By combining above mentioned two results, it is possible to develop a new platform in which *synergistically* will be integrated an optically stimulated enhancement of fluorescence, to the photo stimulated drug delivery systems, that offer the possibilities of the controlled delivery and release of a wide variety of drugs into the body, at the suitable time and desired site, to simultaneously visualize and fight different kinds of diseases including cancer diseases.

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NEAR INFRARED VISUALIZATION OF PROSTATE CANCER CELLS USING GOLD NANORODE CONJUGATED FLUORESCENT DYE COMPLEX

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Gold nanorods (GNRs) functionalized with fluorescent dyes offer a number of properties which make them suitable for use in biological applications, in particular in the diagnosis of diseases such as cancer. Molecular imaging techniques capable of good penetration depth in living tissue remain an important challenge in basic and clinical science, including modern biology and medicine [1 – 3].

In the present work, we propose an in vitro demonstration of GNRs conjugated with near-infrared (NIR) fluorescent dye complex, as an effective contrast agent for the visualization of prostate cancer cells. In this type of imaging, NIR dye / GNR complex is introduced into the subject, which is then exposed to an external source of invisible NIR light that can penetrate the biological tissue. When the light reaches the NIR dye / GNR complex, the dye emits a light which is then picked up by a detector or camera. Thereby we have experimentally demonstrated that:

1. NIR dye / GNR complex is prone to distribute across the location of the prostate cancer cells (suspected areas were predetermined by Histo-morphological investigations).
2. GNRs can dramatically enhance the NIR light intensity of nearby fluorescent dye because of the interactions between the dipole moments of the fluorescent dye and the surface plasmon field of the GNRs. Similarly to the work [4], we have found that the electric charge on the GNRs and the distance between GNRs and dye molecules have a significant effect on the fluorescence intensity, and this enhancement depends strongly upon the excitation wavelength of the pumping laser source. Enhancement in luminescence using fluorescent dye/ GNRs complex will lead to many applications for advancement in biomolecular labeling to produce novel optical contrast agents with high sensitivity and specificity. This method can be highly advantageous for the early stage cancer detection and visualization, because the reduced scattering and absorption of NIR irradiation (750 – 900 nm), which results in a deep penetration of light in the biological tissues.

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METAL NANOPARTICLE PRODUCING BASED ON ELECTRO-PHYSICAL METHODS

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Properties of nanoparticles are largely dependent on technology for their producing. In this regard, special place is occupied by electro-physical methods (EPM) of metal nanoparticles (MNP) generation. EPM principle is based on the electrical conductivity of metals and, in this paper, experimental results of particles generation both pulsed and continuous regimes are considered.

MNP are characterized different degrees of bacterial activity. Most using in practice had got silver, copper, zinc, gold. In particular, nanoparticles of copper have is shown high germicidal and bacteriostatic efficiency, given the relatively low cost of copper compared with noble metals used in pharmacology, makes the prospects of its use [1, 2].

There are two modes of EPM in which correspondingly two ways of the MNP formation are realized. In first one the MNP are produced as a result of dispersing macroscopic initial metal pattern. Such a mode of pulse regime is realized at electric explosion of wire (EEW) or foil [3 – 5]. EEW effect does not depend on properties of the medium in which the explosion take place, so in the experiments, a container where EEW was realized filled with distilled water or air [6]. If explode the wires of different metals one can get the mixed powder [7].

The MNP produced as a result of EEW effect have got size distribution close to lognormal [8]. Significant positive feature of the EEW consist in possibility to control of characteristic size and width of distribution by means of control of electric circuit parameters. Experimental laboratory equipment was designed and the results of investigation of copper nanoparticles biologic activity are presented.

Another method of MNP producing based on the high aggregation activity of metal nanostructures. The single atom is lowest size limit of nanoparticle. Therefore, by generation of atoms of the metal and creating the condition for their aggregation we can produce MNP with preassigned size. The structural scheme of the experimental equipment based on Gen–Miller magnetic-levitation melting of metal is designed and discussed [9].

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FORMATION OF INDUCED ANISOTROPY IN COMPACTED CHROMIUM DIOXID NANOPOWDERS

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Magnetoresistive and magnetic properties of compacted powder of ferromagnetic half-metal CrO_2 with a Curie temperature $T_C \approx 390$ K was studied. A chromium dioxide powder was made by hydrothermal synthesis [1] and consisted of acicular CrO_2 particles with mean diameter ~ 24 nm and length 302 nm. CrO_2 particles were coated with ~ 1.3 nm in thickness dielectric layer made of naturally degraded non-magnetic material β-CrOOH. The sample was prepared by cold pressing of the obtained CrO_2 powder with dielectric coatings in the form of parallelepiped with dimensions $3 \times 5 \times 12$ mm^3. β-CrOOH provides tunneling of electrons between the conducting ferromagnetic CrO_2 granules. In macroscopically isotropic material we found quite a large anisotropy of the tunneling magnetoresistance (MR) associated with the orientation of the magnetic field relative to the axis of pressing. The magnitude of the MR anisotropy significantly exceeded the expected contribution of the spin-orbit interaction, which for bulk ferromagnets usually does not exceed (1 – 2) % [2]. But for the studied sample the maximum value of anisotropy, accounted for as $A(H) = [R(H_{||}) - R(H_{\perp})]/R(0)$ achieved 15.7 % at T = 4.2 K. Here $H_{||}$ and $H_{\perp}$ are longitudinal and transverse magnetic fields, respectively.

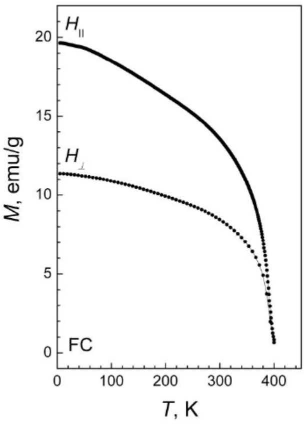

Figure 1.

Magnetic measurements showed that the sample has an induced magnetic anisotropy (see the **Figure 1**) presumably related to the formation of the texture in the magnetic powder during compression. Electron microscopy studies show that needle-shaped CrO_2 particles are mainly oriented in the sample plane which is perpendicular to the axis of the sample pressing. In this orientation, the projection of the particles' light magnetization axis c on the direction of the external magnetic field is substantially larger for a longitudinal field $H_{||}$, which leads to a higher value of sample magnetization M in this direction. Magnetization hysteresis measurements showed that the magnitude of $\mathrm{d}M/\mathrm{d}H$ is higher for a longitudinal field. This means that the demagnetizing factor in the field $H_{\perp}$ is higher than in $H_{||}$.

Thus, in powders of uniaxial magnetic CrO_2 while pressing the material the magnetic anisotropy is induced. This leads to anisotropy of tunnel MR in macroscopically isotropic system. Our studies have shown that the anisotropy of the nanoparticles' form allows you to create magnetic nanostructures with the preferred orientation of the magnetic moments parallel to the axis of symmetry of the nanoparticles, which significantly changes the magnetic properties of the material and the magnitude of tunneling MR. Thus, by controlling the anisotropy of the form of nanoparticles, it is possible to control the process of magnetization and magnetoresistive properties.

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THE ELECTROCHEMICAL METHOD PRODUCING GRAPHENE OXIDE AND REDUCED GRAPHENE OXIDE FROM MULTIWALLED CARBON NANOTUBES

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Graphenes are the promising electrodes material for electrochemical power generators [1 – 5]. From the analysis of the standard redox potential of carbon in acidic and alkaline solutions were chosen the required potentials [6 – 8] for the electrochemically obtaining by oxidation of carbon the graphene oxide (EGO) (**Figure 1**) and the electrochemical reduction graphene oxide (ERGO) (**Figure 2**). EGO was obtained by anodic oxidation of multiwalled carbon nanotubes (MWCNTs) in a specially designed cell in a concentrated solution of sulfuric acid at a potential of 3 V for a few hours. The ERGO was obtained by cathodic reduction EGO in alkaline solution at a potential of – 1.8 V for a few hours. To prove that the obtained materials from MWCNTs by proposed electrochemical method are the graphenes were used electron microscopy, XRD analysis and Raman spectroscopy. From this materials used as active layer were made oxygen electrodes. Then these electrodes have been investigated in the mock up of the fuel cell. It is found that these materials are electrocatalytically active in the reaction of oxygen reduction, and are stable during the semi-annual tests. The resulting catalytic activity in the reaction of oxygen reduction shows that the electrochemical method is very good for producing graphene materials for the electrodes of power sources.

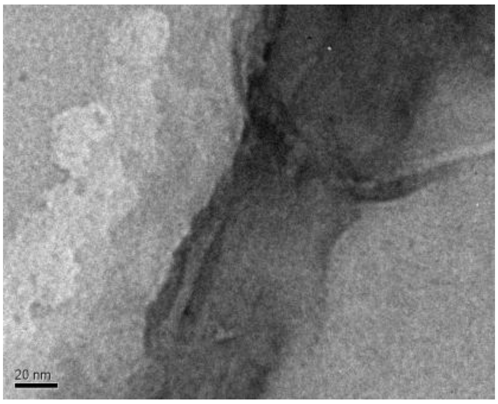

Figure 1. Electrochemical graphene oxide.

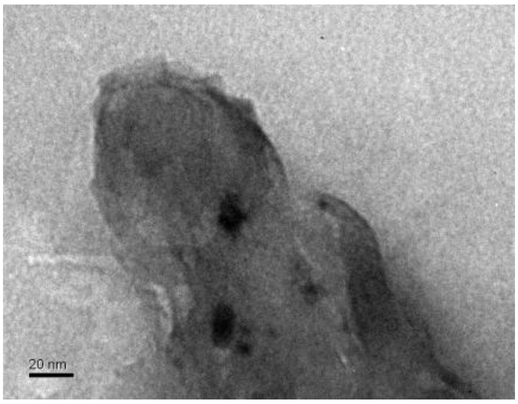

Figure 2. Electrochemical reduced graphene oxide.

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INFLUENCE OF ELECTRIC FIELD ON THE INFORMATION CHARACTERISTICS OF FILMS OF POLYAZOBENZENE AND THEIR METALLOCOMPLEXES FOR POLARIZATION HOLOGRAPHY

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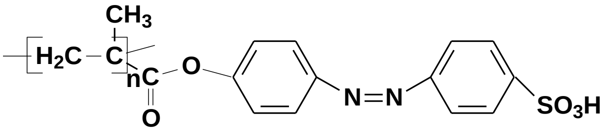
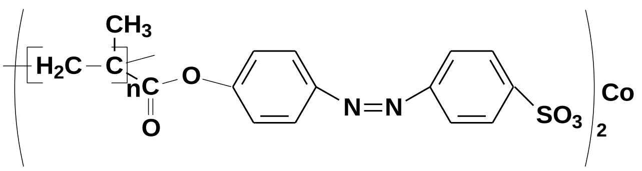
The films of azobenzene polymers and their metallocomplexes can be employed [1 – 3] as electrooptical modulators and in recording media for polarization holography (HRM). This work is devoted to investigation of the possibilities of influence of external electric field on the properties of polarization sensitive holographic recording media. HRM based on the films of new azobenzene polymers poly-AZO-S and poly-Co-(AZO-S)$_2$ were synthesized:



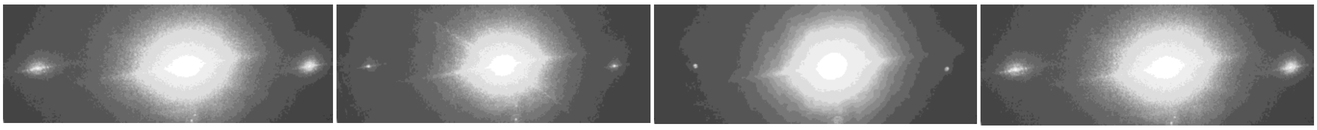
poly-AZO-S



poly-Co-(AZO-S)$_2$

The HRM samples were prepared as polymeric films deposited from solutions onto the glass substrates with transparent conducting layer SnO_2 : In_2O_3. This layer was employed as the electrode for formation of the electric field in the films by crown discharge. Decrease of the diffraction efficiency of the recorded in investigated HRM holograms was registered after application of electric field. The holograms of flat wave front were registered using semiconductor laser with λ=532 nm.

Figure 1 demonstrates screen with images of reflected beams after recording of hologram in HRM with poly-AZO-S (a) and next after 5 s (b) and 60 s (c) after application of external electric field $E \cdot 10^8$ V/m. When E is switched off the intensity of diffracted light restores (d).



(a) **(b)** **(c)** **(d)**

Figure 1.

HRM with poly-AZO-S is characterized by lower noise level as compare to poly-Co-(AZO-S)$_2$ due to its higher homogeneity. Nevertheless, presence of Co ions can essentially improve the HRM information characteristics. The phenomenological model describing the mechanism of the field E effect on the diffraction efficiency of polarization holograms is proposed.

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PHOTOCONDUCTIVITY OF FILM POLYMERIC COMPOSITES WITH PARTICLES OF COMPLEXES Cu (II) / Mo (VI)

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The films of polymeric composites (FPC) containing heterometallic complexes are considered as the media for information technologies and photoelectric converters due to inner photoeffect observed there [1, 2]. Photoconductivity of such FPC is attributed to optical $d-d$-transitions in metallic ions and electron transfer inside the complex particles and between them. The photoconducting properties of FPC based on non-photoconducting polyvinylbutyral (PVB) doped with particles of complexes $(NH_4)_{2n}\{[Cu(en)_2][Cu(en)(H_2O)][P_2Mo_5O_{23}]\}_n \cdot 3nH_2O$ (K1) and $(NH_4)_{4n}\{[Cu(en)(H_2O)][P_2Mo_5O_{23}]\}_n \cdot 3.5nH_2O$ (K2) were investigated (en is ethylenediamine). In the samples of sandwich-structure ITO–(PVB + 50 mass % K1)–Ag, ITO–(PVB + 50 mass % K2)–Ag after start of illumination with light from absorption range of Cu (II) from the side of transparent electrode ITO the current of conductivity increases and after certain time (60 ± 5 s for the samples with K1, 35 ± 5 s for the samples with K2) reaches quasi-stationary value j_{PHmax}. Kinetics of the photocurrent after light switching on and its ceasing is symmetric. Influence of electric voltage U, light intensity I, and temperature T on j_{PHmax} is investigated. The main results can be described by dependency $j_{Phmax} \sim I \cdot U^m \exp(-W_{aPH}/k_B T)$, where m is the exponent of volt-ampere characteristics, W_{aPH} is the activation energy of photocurrent, k_B is the Boltzmann constant.

In all samples $|j_{PHmax}|$ is proportional to I and does not depend on U polarity. However, for the same values I and U the value $|j_{PHmax}|$ is larger in the samples with K2 as compare to the samples with K1. In the samples with K1 and K2 values m and W_{aPH} are also different: in samples with K1 $m = 2.0 \pm 0.1$, $W_{aPH} = 0.75 \pm 0.02$ eV, in the samples with K2 $m = 1.4 \pm 0.1$, $W_{aPH} = 0.40 \pm 0.02$ eV. Before developed model considerations about the mechanism of photogeneration, recombination, transport and capture on energetic traps of non-equilibrium charge carriers were used for explanation of the experimental results. Accordingly to these consideration electronic transitions between metallic centers occur after light absorption in the particles K1 and K2. In the external electric field non-equilibrium charge carriers move toward the accumulating electric contacts inside these particles and between them through neutral PVB. Growth of $|j_{PHmax}|$, decrease of the photoresponse time, decrease of m and W_{aPH} in the samples with K2 is attributed to improvement of transport conditions for non-equilibrium charge carriers in the particles K2. Results of present investigations can be useful for development of new photoconducting FPC with metallocomplexes.

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FLUIDS DYNAMICS IN THE VICINITY OFFERROMAGNETIC SOLIDS UNDER THE INFLUENCE OF A DC MAGNETIC FIELD

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The study of the interaction of metal surfaces with electrolytes under the influence of an external magnetic field and the autocatalytic formation of spatiotemporal structures are of great interest in the recent years. The magnetic field in this case is an additional parameter that allows us to modify existing or create new structures by changing or substitution of reaction mechanisms. The measurements of the dynamic characteristics of the motion of fluids are caused by the need to enter marker particles in the medium under investigation or usage other mechanical methods. The proposed method of obtaining data on the motion of fluids does not require the use of additional inclusions and allows us to avoid the distortions caused by such inclusions.

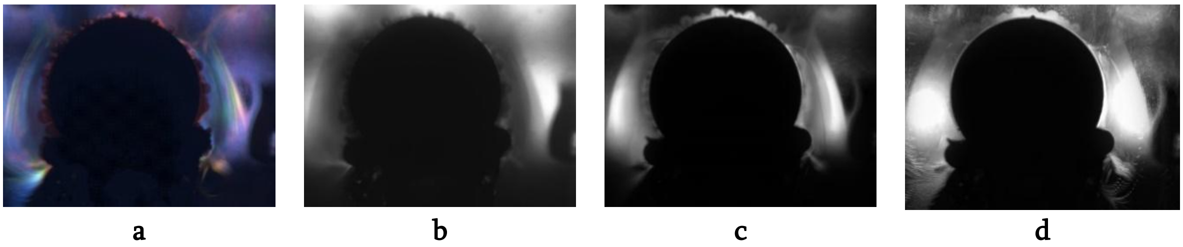

Figure 1. Electrolyte vortexes frequency distribution visualization: a) summary image (red colour corresponds to the frequencies 0.05 – 0.5 Hz, green colour – 0.5 – 2.0 Hz, blue colour – 2.0 – 15 Hz); b) averaged image; c) dispersive image; d) normalized image.

We used the medium similar to that used in Ref. [1] as a model one as the magnetic field applied to it allows to stimulate the autocatalysis of the reaction. Due to arising of such structures, the refractive index and the optical transparency of the electrolyte change. Because of the fact that the intensity and distribution of the magnetic field does not change during the reaction, the dynamics of the change in phase distribution of the electrolyte is caused by the changes in acid and reaction products concentrations, and, consequently, by the mechanism of the reaction. The statistical characteristics, in contrast to integral ones, do not give information about the characteristic frequencies of the electrolyte flows, but show their configuration and intensity (**Figure 1**). As a whole, by using these characteristics we can make conclusions on both reaction mechanisms and sites of its maximum and minimum intensities. It allows both to study the peculiarities of the reaction and to determine corrosion areas of metallic compounds in terms of dynamical characteristics of electrolyte. In general, the developed method allows us to obtain the distributions of the characteristic frequencies of the motion of fluids, gases, and small objects over the volume of the medium under investigation without a direct influence on this medium.

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GOLD MICRO AND NANO PARTICLES FOR SURFACE ENHANCED VIBRATIONAL SPECTROSCOPY OF PYRIDOSTIGMINE BROMIDE

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Nanosized particles of noble metals can work as an optical antennas enhancing spectral signal from the analyte molecules adsorbed on it. This effect is actively used in Surface Enhanced Raman Scattering (SERS) [1] and Surface Enhanced InfraRed Absorption (SEIRA) spectroscopies [2].

Triangular gold microprisms and spherical silica core-gold coat nanoparticles were examined by us as active nanostructures for the surface enhanced Raman and infrared spectroscopy. These particles were probed for the detection of pyridostigmine bromide as a safe antidote of military sarin gas. Raman and infrared spectral bands of the pyridostigmine bromide were measured. Detailed correlation of obtained spectral bands with specific vibrations in pyridostigmine bromide was done. Silica core – gold coat nanoparticles showed more essential enhancement of the Raman signal than gold microcrystals.

Here we show that gold coats are more effectively enhance Raman and infrared signals than gold microcrystals. Particularly Raman signal from pyridostigmine bromide deposited on the silica core-gold coat nanoparticles is enhanced in 50-100 times in comparison with the same substance deposited on glass. This enhancement is connected with more effective excitation of plasmons localized in gold nanocoats. The strongest Raman and infrared spectral bands are detected in the spectral range 1000 – 1200 cm^{-1} and connected with C–N stretching vibrations of the tertiary amine in the pyridostigmine molecule.

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GRAPHENE SUPPORTED CERIA – THE NEW PERSPECTIVE CATALYST FOR NON-DESTRUCTIVE TRANSFORMATIONS OF OXYGENATES

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Graphene-supported cerium oxide has very recently been the focus of much interest as nanocatalysts due to a synergetic effect [1] Attractive prospects are also in the related sensor technology [2]. Ceria was deposited on graphene, using a chemically simple method. The H_2-TPR measurements and HRTEM, textural and Raman studies were performed. The results were promising, confirming high activity of the material having sufficiently uniform distribution of CeO_2 indicating high catalytic activity.

The catalytic high temperature transformations of ethanol and butan-1-ol under anaerobic conditions, i.e. without the participation of molecular oxygen but with participation of oxygen functional groups allowed dehydrogenation and consecutive bimolecular condensation reactions to form esters (Tishchenko reaction) and symmetrical ketones containing $2n-1$ carbon atoms in chains [3]. Depending on the control parameters, ethyl acetate and propan-2-one or butyl butanoate and heptan-4-one can be efficiently obtained. This kind of transformations of oxygenates concern primary alcohols, aldehydes or esters (ketonization only). The gas phase catalytic synthesis can facilitate production of fine-chemicals. Due to the competitive dehydration, few catalysts are able to perform the above transformations. The hybrid component was synthesized with goal of achieving an analog of carbonaceous active phase [4].

Application for a Polish–Ukrainian. Joint Research Project for years 2015–2017, Polish Academy of Sciences and National Academy of Sciences of Ukraine: Hybrid graphene nanomaterials for catalytic applications.

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ACOUSTIC DETECTION OF RESONANCE PLASTICIZATION OF LiF CRYSTALS UNDER THE EFFECT OF CROSSED MAGNETIC FIELDS IN THE EPR SCHEME

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The authors of work [1] were the first to predict theoretically and the authors of work [2] – to show experimentally that the joint action of crossed permanent $B_0$and high-frequency (HF) $B^{\sim}$ magnetic fields could lead to resonance plasticization of nonmagnetic crystals when frequencyν of the HF field satisfies the condition of electron paramagnetic resonance (EPR) $h\,\nu = g\,\mu_B\,B_0$, where h is the Planck's constant; g is the Lande factor; μ_B is the Bohr magneton. In this work the experimental results on the effect of crossed magnetic fields in the EPR scheme on the dislocation internal friction of LiF crystals are discussed. The preliminary experiments, carried out by the method of microindentation, showed that, in the LiF crystals under studyin crossed magnetic fields in the EPR scheme, the resonance displacement (depinning) of dislocations occurred. The effect was maximum at the frequency of 9.525 MHz which satisfies the condition of paramagnetic resonance at $g=2$ ($B_0 = 340$ μT, $B^{\sim} = 10$ μT); the frequency of the HF field varied in the interval from 9.2 to 9.8 MHz. These data were used when performing the acoustic measurements.

Before the measurement, fresh dislocations were introduced into the sample (10 indentations under the load of 2 N). With small amplitudes of deformation of about 10^{-5} (amplitude-independent internal friction), forced oscillations of the crystal were excited (at ≈ 3 kHz) (**Figure 1**), and the post-deformation internal friction return was registered. If, at this moment we subjected the sample to the effect of crossed magnetic fields with the frequency of $\nu = 9.525$ MHz, we would observe an internal friction jump. The effect is irreversible: the crystal did not respond to the repeated switching on / off of the fields. To observe the jump again, it was necessary to introduce fresh dislocations by indentations.

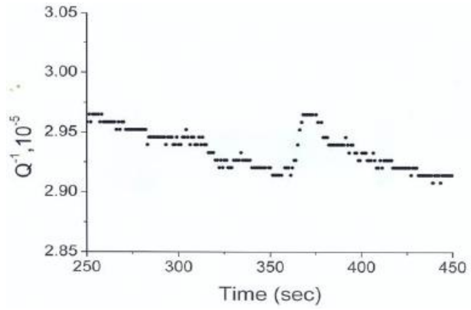

Figure 1.

From the results of preliminary experiments, it is obvious that the observed increase in mechanical energy dissipation was caused by breakaway of dislocations from pinning centers, induced by the magnetic field. The physical cause of the effect is the structural deformation of impurity centers in the dislocation-impurity nanoreactor in the result of paramagnetic resonance.

Thus, the possibility of acoustic detection of resonance plasticization of nonmagnetic crystals under the effect of crossed fields in the EPR scheme is shown for the first time.

The work is supported by AFOSR bygrant ISTC–G1966P and by grant FR/144/6-130/13 of Shota Rustaveli National Science Foundation.

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ORGANIC–INORGANIC HYBRID MATERIALS AS CATALYSTS FOR FINE ORGANIC SYNTHESIS

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Recently, the industrial production of fine chemicals using "green" and other resource-saving technologies has become of special importance. From this perspective, heterogeneous catalysis is one of the most promising processes that can replace traditional chemical technologies causing significant environmental damage. Periodic surface structure of mesoporous silica is a great advantage to implement a structured orientation of guest molecules in the pores, resulting in the increased selectivity and activity in catalysis [1]. For practical application, hydrothermal resistance of materials is very important. This is due to the fact that most acid-catalyzed reactions, such as esterification, hydration, and condensation occur with the participation of water. Incorporation of sulfonic acid in the structure of mesoporous organosilica is especially interesting, because organic bridging group can provide hydrophobicity of the materials and, thereby, ensure their hydrothermal stability for the use in catalysis. What is more, such samples can be offered for possible use as solid acid catalysts, adsorbents for chromatography, nanofillers in fuel cells, and as sorbents of trace concentrations of certain metal ions [2 – 4].

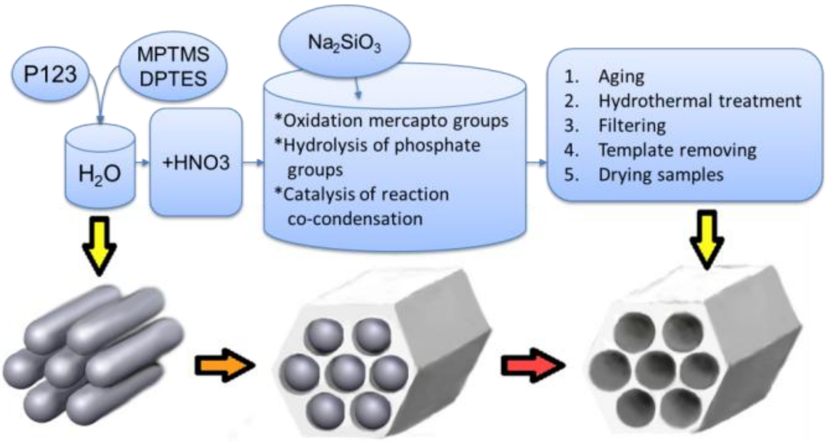

Figure 1. Scheme of template synthesis. Notes: P123 – pluronic 123, $EO_{20}RO_{70}EO_{20}$, poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide); Na_2SiO_3 – sodium metasilicate $Na_2SiO_3 \cdot 9H_2O$; DPTS – diethylphosphatoethyltriethoxysilane $(C_2H_5O)_3Si(CH_2)_2P(O)(OC_2H_5)_2$ MPTMS – 3-mercaptopropyltrimethoxysilane

Given the high reactivity of phosphonic groups, there is a high probability that the synthesized bifunctional catalysts would possess higher capacity compared to monofunctional sulfo-containing product (**Figure 1**).

O. A. D. thanks Fulbright Scholar Program for the financial support of the present work (Grant ID 68120263, 2012 – 2013).

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EFFECT OF THE SUBSTITUENTS UPON THE PHYSICO-CHEMICAL PROPERTIES OF SILICA XEROGELS

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Developing and application of suitable host materials for biomolecules or bioactive substances (drugs) or sensitive organic dyes is a challenging task for current organic and inorganic chemistry. The ambient processing conditions, flexibility and versatility of the sol–gel method makes the sol–gel silica matrices suitable host materials for such molecules.

The present study focuses on the synthesis and physicochemical characterization of methyl and vinyl substituted silica gels prepared using different amount of the substituent molecules. Also the catalysts type and quantity has a strong effect on the properties of the resulted silica host materials. The texture, morphology, chemical composition and thermal stability of the hybrid materials were characterized by nitrogen adsorption, small angle neutron and X-ray scattering; electron microscopy (SEM and TEM); FT–IR and ^{29}Si–MAS–NMR spectroscopy; and thermal analysis.

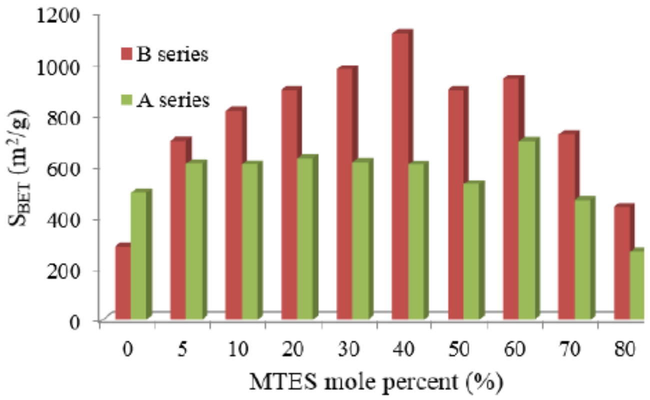

Figure 1. Specific surface evolution:
A – NaF and B – NH_4F catalysts.

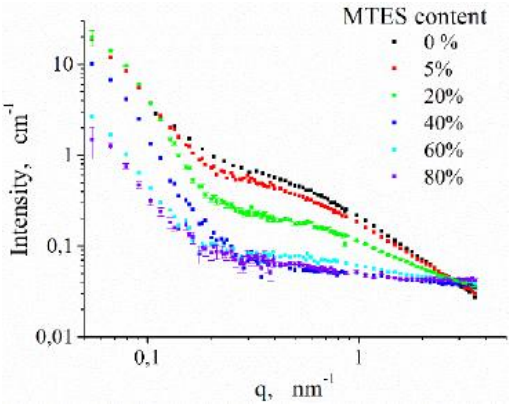

Figure 2. SANS scattering
curves for series A

All the presented xerogels show lamellar and porous structure with very high, up to 1000 m^2 / g surfaces (**Figures 1** and **2**). The hydrophobicity and the degree of condensation are increasing with amount of added substituent. In this study we attempt to provide a better understanding of the silica structure modification with the methyl or vinyl substituents, using different amount and type of the catalysts. With the modification of the precursors, catalysts quantity the hydrophobicity, porosity and biocompatibility of the synthesis condition can be adjusted for the desired applications.

GROWTH AND CHARACTERIZATION OF III–N ULTRAVIOLET LASERS AND AVALANCHE PHOTODIODES BY MOCVD

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The field of ultraviolet (UV) photonics at wavelengths $\lambda < 400$ nm is an area of increasing practical interest and coherent light sources and fast, sensitive photodetectors are needed for many important applications. In this study, AlGaN p-i-n APDs are demonstrated on “free-standing” (FS) n-type (0001) GaN substrates having low dislocation densities. The AlGaN PIN UV–APDs and UV lasers were epitaxially grown on a *c*-axis n-type free-standing GaN and sapphire substrates using metalorganic chemical vapor deposition (MOCVD). For top-illuminated APD structures, step-graded layers from n-GaN : Si to $Al_{0.02}Ga_{0.98}N$: Si were introduced instead of a single n-$Al_{0.05}Ga_{0.95}N$: Si layer as a strain management scheme for crack-free growth.The APD epitaxial layer structure consists of a 0.45 μm thick GaN : Si layer followed by a 0.15 μm thick *n*-$Al_{0.02}Ga_{0.98}N$: Si layer for the step grading, a 0.3 μm thick unintentionally-doped $Al_{0.05}Ga_{0.95}N$ layer, a 0.1 μm thick $Al_{0.05}Ga_{0.95}N$: Mg layer, and a 0.02 μm thick $Al_{0.05}Ga_{0.95}N$: Mg^{++} grown on FS-GaN. The growth and doping conditions for epitaxial layers were optimized to achieve improved crystalline and structural quality by modifying the MOCVD growth parameters. The APD wafers were fabricated into circular mesas with various diameters using standard photolithography and inductively coupled plasma etching, followed by SiO_2 passivation deposited using plasma-enhanced chemical vapor deposition. The APDs exhibit a maximum avalanche gain > 10^5 at a reverse bias of 102 V. We have also fabricated UV optically pumped InGaN / AlGaN MQW lasers at 375 nm employing an AlGaAs – GaAs 40 pair n-type bottom DBR operating pulsed at 300K, and will describe the growth, processing, and output characteristics of these lasers.

CALCINATED ZnO NANOPARTICLE: AN EFFECTIVE HETEROGENEOUS NANOCATALYST FOR THE SYNTHESIS OF 10-IMINO-1,3-THIAZOLO [3,4-c]PYRIMIDO[1,2-a]PYRIMIDINE-2,4-DIONE DERIVATIVES

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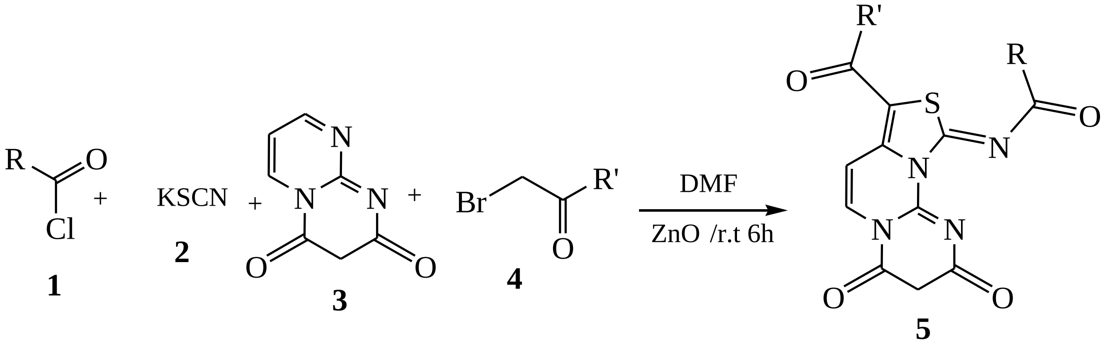
Heterocycles with nitrogen group are a main piece of natural and unnatural compounds with significant biological activity. Pyrimidine derivatives are very important because of having pharmacological activity. Pyrimidine is found in often natural products and pharmaceutically active compounds as significant alkaloids. Main number of their applications has been developed at the laboratory and industrial level. ZnO nano structure is a non-hygroscopic, cheap and non-poisonous compound, which was employed as a catalyst in organic compounds synthesis.



Scheme 1

Herein, we study an efficient synthesis of thiazolopyridopyrimidine derivatives 5 using the reaction of acid chlorides 1, potassium thiocyanate 2, pyrimido 3 and alkyl bromide 4 in the presence of catalytic amount of calcinated ZnO nanoparticles (10 mol %) in good yield (**Scheme 1**).

INFLUENCES OF GOLD NANOPARTICLES ON CHARACTERISTICS OF BONE MARROW MESENCHYMAL STEM CELLS

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In the field of biomedicine, gold nanoparticles (Au NPs) are frequently used for cancer targeted imaging and therapy [1]. These emerging applications are based on introduction of certain amounts of Au NPs into living cells. The optimum quantity of Au NPs is defined by the balance between pronounced direct effect and low side effects like unwanted cytotoxicity [2]. We performed a study of the impact the different concentrations of Au NPs have on both morphological properties of bone marrow mesenchymal stem cells (MSCs).

Au NPs of 15 nm in average were obtained by citrate synthesis [3]. Aqueous solutions with Au NPs concentrations of 1.5, 6, 9 μg / ml were added to MSCs by a passive diffusion. MSCs were cultured in IMDM with 10 % FBS for 14 days. Localization of Au NPs was evaluated by Confocal Laser Scanning Microscopy (CLSM), while the IR spectra were acquired in reflection mode by using a FTIR microscope. IR marker bands (amides, hydrocarbons, etc.) were carefully analyzed.

CLSM allowed to reveal that Au NPs partially localized in the cytoplasm and nucleus (**Figure 1**). During MSCs culturing the heterogenity of adhesive cells decreased with formation of fibroblast-like morphology as it has been examined by optical microscopy. The organization of the cell cytoplasm, shape and size of cells did not change. The dynamics of culture growth in the control and groups with AuNPs at concentrations of 1.5, 6 and 9 μg / ml was similar, but it differed in a rate **Figure 1**. Adding of AuNPs at concentration of 1.5 μg / ml did not lead to significant changes in the studied index during the entire period of observation.

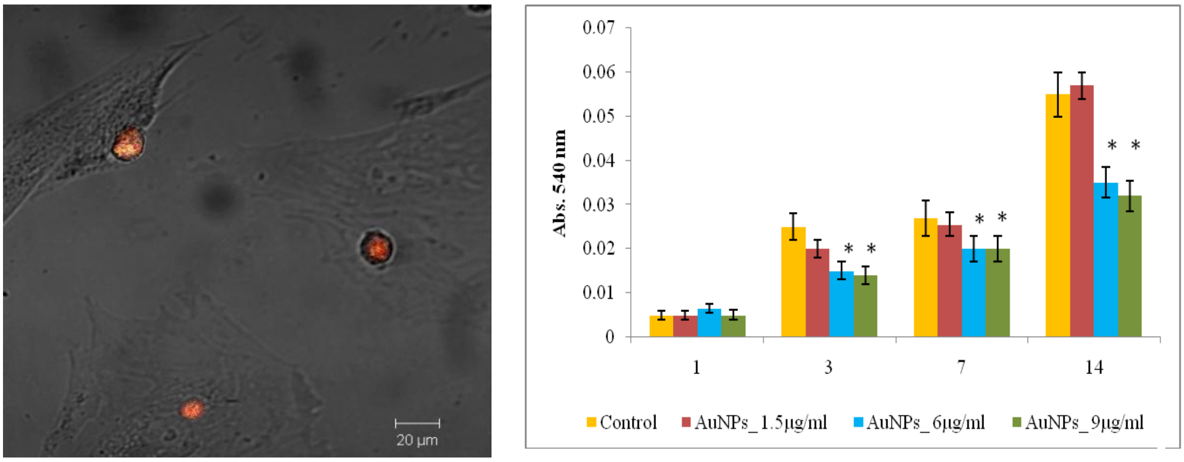

Figure 1. CLSM image of MSCs cells cultured for 7 days with Au NPs of 6 μg / ml (left) and histogram of proliferative ability of MSCs cultured with addition of Au NPs (right).

Intensities of IR marker bands (νN–H, νC–H, Amide I and II) for MSCs with Au NPs were analyzed. The Amide I / Amide II ratio rises with increasing concentration of Au NPs, hence, evidencing the occurrence of apoptosis in the cells under study. There is also an increase of νCH_2 / νCH_3

(asymmetric stretching mode) ratio over the time of cell culturing, which implies the cell growth. Excluding the control sample, there is a trend for almost exponential growth of νCH_2 / νCH_3 ratio with increase of Au NPs concentration (**Figure 2a**). Opposite to this, ratio of νCH_2 / νCH_3 peak area is decreasing with rise of Au NPs quantity (**Figure 2b**). The observed changes in IR bands can be attributed to the expanding proportion of phospholipids in biomass.

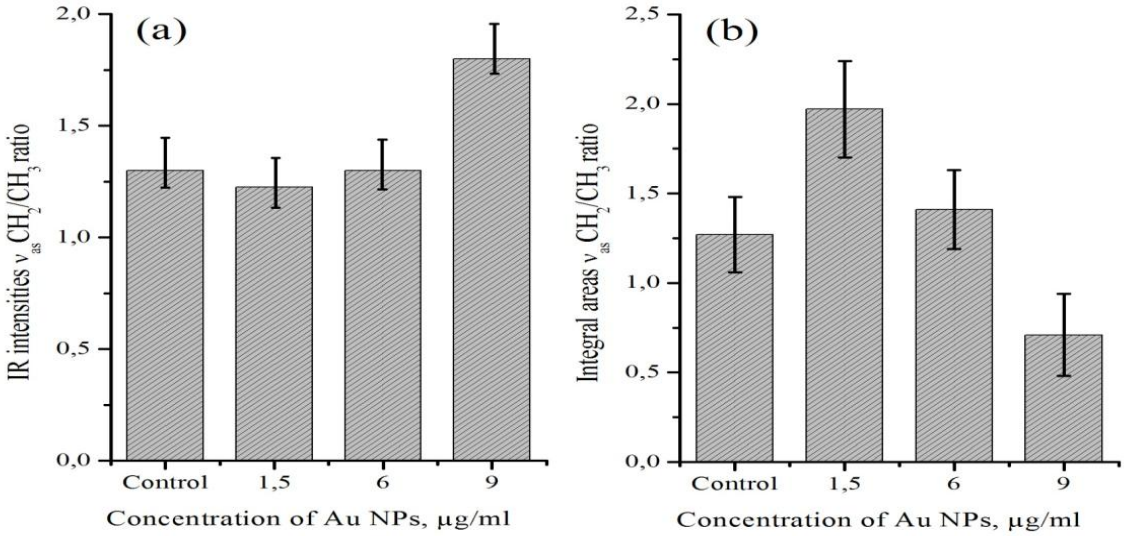

Figure 2. Ratio of IR intensities of asymmetrical CH_2 / CH_3 stretching modes (a) and ratio of their integral summations (b) measured on MSCs after cultivation with Au NPs of different concentrations.

It was found that Au NPs concentration of 1.5 μg / ml is save for MSCs, while increase to 6 – 9 μg / ml has a toxic effect, manifested in the reduction of proliferative activity and apparent apoptosis. These findings relate to applied nanotechnology in its extension to clinical medicine, where the addressed drug delivery to affected cells is studied.

The work was carried-out within the research project of targeted complex program of basic research of the National Academy of Sciences of Ukraine “The fundamental problems of creation of new nanomaterials and nanotechnologies”.

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SIZE DISTRIBUTION OF FINE BUBBLES BY INTERACTIVE FORCE APPARATUS

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Fine bubbles mean nano to micro air bubble in the solution and are studied extensively in recent years. Fine bubbles have various special qualities, souse of fine bubbles in many industries is expected. It is expected that in the future fine bubble market will grow up in the world. However, measurement techniques of particle size distribution of fine bubbles haven't perfectly developed yet.

On the other hands, Interactive Force Apparatus (IFA) has been developed so far in our laboratory. IFA is a direct measurement technique, not depending on the concentration and optical transparency. In this point, this technique has advantage to other measurement techniques. This apparatus can measure nano to micro size solid particles and emulsion. Thus, in this study we measured particle size of fine bubbles by IFA and compared the results with ones measured by Dynamic Light Scattering (DLS). Moreover, we made calculation model of interactive forces in a line of chain construction, and compared distribution given by calculation interactive forces with true distribution and results measured by IFA.

In measuring particle size distribution of fine bubbles by IFA, the cycle of repulsive force and attractive force working between hemisphere and flat plate wasn't measured in case of measurement blanc water or measurement under non-electric field. The sample in which fine bubbles were generated using air on 0.2 MPa for 10 min was measured by IFA and DLS, and particle size distributions were resembled closely. In IFA measuring, d50, d25 and d75 were 189 ± 56 and 137 ± 42 nm, and in DLS measuring, d50, d25 and d75 were 182 ± 27 and 133 ± 10nm.

The particle size distribution measured by calculation interactive forces using a line of chain construction model and true distribution given by log normal random number resembled closely.

USAGE OF POTENTIAL INTERACTIONS OF PARTICLES FOR SEARCHING AND CATEGORIZING TEXTUAL INFORMATION

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It is well known that many physical laws find their application in economy, so it's proved for programming and computer science [1]. Articles withtextual informationcan be representedas a formof elementary particles.We find keywords for each article and allocate certain weights for them by using Okapi Bm–25 [2] metric. So, we've got elementary particles with numerical characteristics, which can be divided into clusters. Among non-hierarchical clustering algorithms there are popular algorithms of k-means family [3]. The algorithms of this family are fairly simple and effectively used in processing of large volumes of data.But for algorithms of this family it is required to set a quantity of clusters that should be produced by the split. We propose using subtractive clustering algorithm [4] to determine the number of clusters and perform splitting of articles into clusters using an algorithm of the k-means family. Subtractive clustering method is based on potential interactions of particles. We choose k-means [3, 4] and k-medoids [5] from k-means family for final clustering and comparative analysis. k-means minimizes the total square deviation of points of clusters from the centres of these clusters. k-medoids is similar to k-means algorithm, butit differs in that k-medoids seeks the centres of clusters at each iteration as medoids of points, not as a mean of points.

A computational experiment by a collection of articles (1264 articles) from the web resource Wikipedia.ru demonstrates that this method using the algorithms k-means / k-medoids and subtractive clustering is suitable for automatic clustering of textual information, but it requires further improvements. In this research quality of clustering was estimated by the following formal criteria: Ratkowsky index [6], Maulik–Bandoypadhyay index [7, 8], Score function [7, 8] and by expert evaluation of conformity of the articles to obtained groups.

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ADHESIVE CONTACT OF ROUGH ELASTIC SOLIDS

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Adhesive contacts are of great interest in a variety of engineering applications. Measurement, theoretical and numerical prediction of adhesion force and real contact area are very important in friction and wear studies. Models of adhesive contact between bodies allow evaluation of contact characteristics.

We propose the model with stochastic surface roughness where roughness is simulated by nonlinear Winkler–Fuss layer [1, 2]. The layer can resist to compressive and tensile (in the case of adhesion) contact stresses. Mechanical properties of the layer are determined by statistical theories of adhesive contact between nominally flat rough surfaces [3 – 5]. Normal and sliding contact of solids is described by nonlinear boundary integral equations with non-monotonic operators [2, 6]. The equations are similar to those of classic unilateral contact problems for elastic bodies with Winkler-Fuss coatings. The boundary integral equations are solved by the method of successive approximations [1, 2].

Solutions of the boundary integral equations determine the reduction of effective thickness of rough layer, contact stresses (normal and shear) and contact regions for the full range of Tabor adhesion parameter. Friction force and its nonlinear dependence on normal force are obtained on the base of numerical calculation for different roughness parameters. Nominal and real contact areas are evaluated. Calculated dependencies of adhesion force on micro and macro parameters of contacting solids are investigated. Adhesive contribution to the total friction force is evaluated for wide range of roughness parameters.

The proposed models are applicable for the contact between rough solids with an arbitrary nominal geometry for a wide range of Tabor parameter.

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ANOMALIES OF THE MECHANICAL PROPERTIES OF LiF CRYSTALS CONTAINING HIGH CONCENTRATION OF THE LEAD IMPURITY

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The mechanical characteristics of alkali halide crystals (AHC) are substantially determined by the type of an impurity and its structural state, depending on the concentration, temperature, preliminary heat treatment (annealing, quenching, etc.), and the ratio of masses and radii of the matrix and impurity ions [1, 2]. In this paper we present results of the study of the mechanical properties of LiF crystals with a wittingly high concentration of the Pb impurity (0.12 mol. %).

In the literature, there is little quantitative data on the effect of impurities on the mechanical properties of the AHC. In the case of LiF crystals, the Pb impurity is of interest, because, due to a considerable difference between the masses of the impurity and basic lattice cations ($M_{\mathrm{Pb}} / M_{\mathrm{Li}} \approx 30$) and different radii of ions (R_{Pb} = 0.175 nm, R_{Li} = 0.155 nm), the solubility of Pb is low, and considerable part of the impurity is present in the crystal in the form of the second-phase particles up to 100 nm in size. Moreover, the samples have no growth dislocations. The above-listed factors determined the nonstandard behavior of the initial LiF crystal at the deformation: besides a high value of the yield stress τ_y (**Figure 1**, Curve 1), spontaneous release of the preferential slip system (**Figure 2**) and double cross slip of screw dislocations was observed.

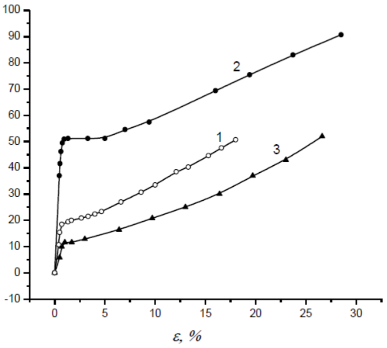

Figure 1.

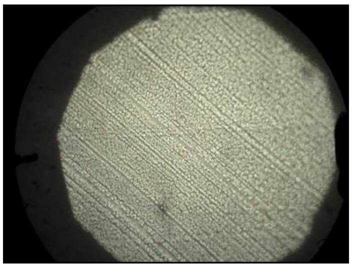

Figure 2.

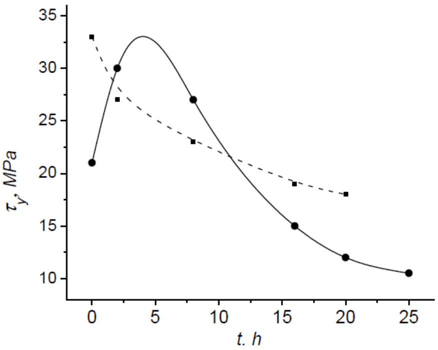

Figure 3.

The response of these samples to heat treatment and irradiation is atypical for doped AHC. Shirt-term high-temperature annealing (800 °C, 1 – 2 h) caused hardening of the crystal (solid curve in **Figure 3**) unlike the crystals with other impurities such as, for instance, Mg (dotted curve). Quenching from the 500 °C (**Figure 3**, Curve 1) decreased the yield stress of the crystal by a factor of three and at the same time plasticized it, which seems to be caused by transition of the Pb impurity from large clusters to a solid solution. The result of irradiation is especially paradoxical: simultaneously with an increase in the yield strength τ_y, high plasticity (up to 30 %) was observed (**Figure 1**, Curve 2), which is not characteristic of AHC that harden and embrittle under irradiation.

The obtained results together with the data on the types of atomic configurations of the Pb impurity and their concentrations at all stages of heat treatment and irradiation allow us to establish the conditions under which we can obtain the crystal with desired anomalously high mechanical characteristics.

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THERMAL EVAPORATION SYNTHESIS OF NANOCRYSTAL PARTICLES

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Isolated nanocrystal particles are usually produced by evaporation of metal at controlled temperature in the low-pressure inert gas atmosphere or in vacuum with subsequent vapor evaporation near a cold surface. In contrast to vapor evaporation, the atoms of the substance evaporated in the rarefied inert atmosphere lose kinetic energy faster by collision with gas atoms and form segregations (clusters) [1]. There are available several versions of the plant for production of nanoparticles [2]. The work deals with the possibility of application of thermal evaporation to the production of nanoparticles. The plant schematic is shown in the **Figure 1**

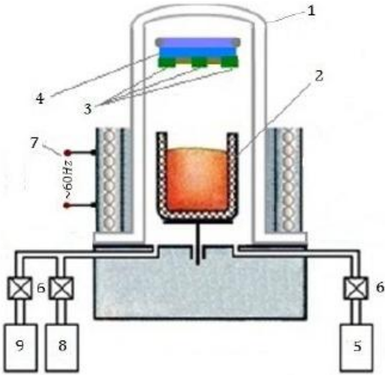

Figure 1. 1 **– reaction chamber housing, 2 – crucible with the sample, 3 – stencil, 4 – substrate, 5 – vacuum pump, 6 – valve, 7 – power supply,** 8 **– bottle with an inert gas, and 9 - bottle with an inert gas-oxygen mixture. The scale is not observed.**

The plant consists of a working chamber, a vacuum system and a control panel. The working chamber (1) is made in the form of a cylindrical cap from quartz (or stainless steel with observation windows). Inside the working chamber, there is a crucible (2), a stencil (3) providing the specified configuration of a layer, and a substrate (4) which the evaporated substance is condensed on. Pumping of the working volume is performed by a vacuum diffusion pump (5) through a hole and a pipeline connected with the pumping volume via a valve (6).

The control panel consists of a power source (7) which heats the evaporating substance [3]. The inert gas rate can be controlled by the readings of the gearbox unit mounted on the inert gas bottle (8). Before opening the plant and taking out the sample, the nanoparticles are passivated by passing an inert gas-oxygen mixture (9) for a few minutes.

The substance is heated for evaporation. The metal to be deposited on the substrate (4) is placed in the crucible (2). The heating effect increases with the increasing field intensity, and depends on the properties of the material and on the distance from the coil to the surface [4].

Being heated, the substance melts and then transfers into a vapor state. When the melted metal vapor in the form of an atomic beam propagates from the melt, the metal atoms transfer from the metal phase to the condensed state, fall on the substrate and deposit on it in the form of a thin film. By varying the evaporation rate, substrate temperature, and gas pressure and composition, nanoparticles can be produced.

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MECHANICAL PROPERTIES OF DYSPROSIUM MONOANTINOMIDE THIN FILMS

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As is known, rare earth elements (RE) antimonides have many unique physical properties, which makes them promising for use in microelectronics, but often, using this material is limited by its low mechanical properties. Since the mechanical properties of antimonide RE thin films have not been studied at all, the study of the mechanical properties of DySb is a very urgent task.

In this paper, for the first time has been studied the dynamic microhardness and indentation modulus of DySb on a sapphire substrate by the method described in [1, 2]. DySb single-phase polycrystalline thin films were prepared using the discrete vacuum-thermal evaporation method of pre-synthesized material. Film thickness was 2.1 μm, they had salt-type cubic lattice with lattice parameter 6.14 Å.

For four values of load 10, 20, 50 and 75 mN dependency, dynamic microhardness (DHV) and indentation modulus (E_{ind}) of the maximum of load ($F_{\max}$) have been explored. The experiments showed that DHV increases almost linearly from 4.2 to 4.5 GPa, also increasing E_{ind} linearly from 3.9 to 4.5 GPa. Based on the data charts, dependencies between dynamics microhardness and indentation modulus of the depth of the load revealed that the DHV, so the Eit increases linearly with increasing depth.

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MICROSTRUCTURE AND MECHANICAL PROPERTIES OF UFG COPPER AT CRYOGENIC TEMPERATURES

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The basic parameters of the microstructure and mechanical properties of UFG oxygen-free copper polycrystalline (Cu-OF), processed by two methods: direct (DE) and equal channel angular hydrostatic extrusion (ECAE) were investigated. The microstructure parameters were obtained using standard electron back scattering (EBSD) and X-ray (XRD) diffraction methods. The yield stress and strain rate stress sensitivity of UFG polycrystals on the temperature were studied at tension and stress relaxation tests in the range of 4.2 – 300 K.

It was found that the increase of yield stress of samples after DE and ECAE may be explained by tree microstructure parameters: grain size d, dislocation density ρ and texture. The first two parameters, $d \approx 500 - 600$ nm from EBSD and $\rho \approx (2.9 - 4.9) \cdot 10^{14}$ m^{-2} from XRD analysis, are comparable for both DE and ECAE samples where texture is strongly depend on processing method resulting on higher yield stress after DE.

Taking into account the role of texture the temperature dependencies of yield stress and activation volume of plastic deformation were analyzed and three rate controlling mechanisms of plastic deformation were proposed to explain the experimental data. In the temperature range 77 – 200 K both dependencies was found typical for the mechanism of thermally activated intersection of “forest” dislocations with the empirical energy parameter ~ 0.52 – 0.54 eV and the activation volume ~ 200 – 500 d^3.

Below 77 K and above 200 K the experimental data were found deviate from “forest” intersection mechanism resulting in two low and high temperature anomalies of activation volume. The low-temperature anomaly (below 77 K) is explained by the thermal-inertial mechanism consisting on the inertial properties of dislocations at large effective stresses and low dynamic friction forces. For this case the inertial unzipping of moving dislocation from local barriers becomes effective.

Above 200 K, the observed decrease of the activation volume with temperature increase is explained by thermally activated bow-out and depinning of dislocations from local obstacles in the grain boundaries characterized by an empirical energy parameter ~ 2.1 eV which no reveals in conventional polycristals but resulting effective for UFG crystals of copper.

C-PHYCOCYANIN (*Spirulina platensis*) AND METAL IONS

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The cyanobacteria cells play an important role in remediation of toxic metals through reduction of the metal ions; these biological systems have been extensively used for the biosynthesis of metal nanoparticles [1]. The application of nanoparticles as delivery vehicles for bactericidal agents represents a new paradigm in the design of antibacterial therapeutics [2]. The presence of metals can have an enhancing effect on pigment content in cyanobacteria cells. Metal exposure can be an interesting method to induce, in microalgae cells, the synthesis of target products such as pigments, lipids, nanoparticles and etc. However, stimulation of target compound production in microalgae depends on many factors such as metal type and concentration or metal combination leading to synergistic effects, etc.

In this work, influence of metal ions on C-phycocyanin (C-PC) from cyanobacteria *Spirulina platensis* is investigated using fluorescence spectroscopy. Fluorescence measurements demonstrate quenching of C-PC emission by metal ions, and blue shifts in the fluorescence spectra. Stern- Volmer quenching constant were obtained from the linear quenching plots.

The binding energies of heavy and toxic metal ions with C-phycocyanin were determined using equilibrium dialysis and atomic absorption spectroscopy. Cooperative binding of metal ions with C-phycocyanin were observed. The binding constants diminished with increasing ionic strength, suggesting an adaptive protective response.

“Nonelectrostatic” and polyelectrolyte component of binding free energy for Ag^{+}, Cu^{2+}, Cr^{3+}, Pb^{2+}, Ni^{2+}, Zn^{2+}-C-phycocyanin (*Spirulina platensis*) complexes were determined. It was shown, that “nonelectrostatic” component of binding free energy is dominating at the metal–C-PC interaction, while the polyelectrolyte contribution being less important and the “nonelectrostatic” forces contribution for Ag^{+}-C-phycocyanin (*Spirulina platensis*) complexes is more than for other metal ions.

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SPIN WAVE LOCALIZATION IN LAYERED MAGNETIC STRUCTURES OF DIFFERENT TYPES WITH NARROW MAGNETIC LAYERS

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In the present study, we describe a magnetic structure with nonlinear characteristics having narrow layers which differ in their magnetic properties from the surrounding matrix. The layered structures of the forms of ferromagnet / ferromagnet, ferromagnet / antiferromagnet, antiferromagnet / antiferromagnet with different magnetic properties of the layers are examples of multilayered magnetic systems of such a type. An example of such a system is the layered ferromagnet / antiferromagnet Co / CoO structures investigated by Stamps et al. [1].

We study analytically the layered easy-axis ferromagnet with different constants of single-ion anisotropy in thin layers and in the areas outside them. For a layered ferromagnet containing narrow magnetic layers (plane magnetic defects) with easy-axis type anisotropy, directed perpendicularly to the layers, we show that the Landau–Lifshitz equation for the magnetization vector in the long-wave approximation can be reduced to a standard nonlinear Schrödinger equation (NSE) with a periodic array of δ-functions containing both linear and non-linear contributions. On the first stage, in the case of a single plane magnetic layer (NSE with single δ-function), which differs only by the value of single-ion anisotropy constant from the magnetic medium in the region outside the layer, we obtain an exact solution in the form of localized soliton state at the interface between the layers. Also we investigate the properties of the found low-amplitude soliton solution.

In [2] it was presented an analytical study of the stability of the solutions obtained for NSE with single δ-function, with different characters of interaction in the system according to the method proposed by Vakhitov and Kolokolov [3]. Based on the results of [2], we investigate the stability of the localized soliton state in the considered multilayered magnetic system and make the conclusion about its stability with respect to small perturbations of the amplitude and phase. The plane magnetic layer effectively attracts the spin waves and is a factor stabilizing the soliton state. At the same time, in accordance with the results of [2], the oscillation mode of soliton's gravity center relative to the plane of the selected layer is present in the spectrum of small excitations of the state localized at the magnetic layer.

The developed theory and derived NSE can be applied for the investigations of localization of spin waves in different types of multilayered magnetic systems or thin films with narrow plane layers which differ in their magnetic properties from the matrix of the system.

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NONLINEAR LOCALIZED STATES AND THEIR STABILITY IN AN ANHARMONIC MEDIUM WITH A THIN NONLINEAR DEFECT LAYER

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Within the framework of the nonlinear Schrödinger equation with δ-functional perturbation containing both linear and nonlinear parts, we study all possible states localized near a thin plane defect layer (interface), for different signs of nonlinearity of the medium and for different characters of the interaction of elementary excitations of the system with the layer. The quasi-classical interpretation of these nonlinear localized modes in terms of bound states of a large number of elementary excitations is proposed. The regions of existence are determined and the properties of such localized states depending on the character of interaction of elementary excitations with one another and with the defect are studied.

Both analytical and numerical investigations of the stability of all found localized solutions relative to small perturbations of amplitude and phase according to the method proposed by Vakhitov and Kolokolov [1] are performed. It is shown that the presence of an attracting defect layer is a factor stabilizing the localized state. In this case, a localized state exists and is stable both for attraction between quasiparticles, and for their mutual repulsion. In the first case (attraction), the oscillation mode of the soliton gravity center relative to a defect is present in the spectrum of small excitations of the localized state, and the frequency of small oscillations of the state localized on the defect layer is found. In the second case (mutual repulsion), such a mode does not exist, and we have only the continuous excitation spectrum. In this case, oscillations of the localized flow relatively to a defect layer are absent, although its localization holds. In the case of a repulsive defect layer (in attractive medium) the localized state is unstable – interface deforms and repels it. Also we performed the stability analysis for the cases of the opposite signs of linear and nonlinear parts of the defect layer.

Thus, we investigated all possible soliton states localized near a thin plane defect layer, describing by both linear and nonlinear terms, and made a complete analysis of stability of these solutions for an arbitrary type of interaction of quasiparticles with one another and with the defect layer.

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LOCALIZATION OF REAL POLYMER CHAINS AT TWO INTERFACES SIMULATED BY NARROW POTENTIAL WELLS

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It is known that the nonlinearity of the medium can give rise to new physical effects such as dependence of the transparency of the medium on the power of the wave being transmitted, spatial localization of nonlinear waves in periodic arrays of optical waveguides, etc. From the point of view of technological applications, of special interest are layered and modulated structures of different types. In nonlinear optics, for example, where layered and modulated structures are used in optical communication systems, photonic crystals, optical delay lines, the investigations of localized states in the system with two linear/nonlinear defect layers and in periodic modulated structures are very actual. Also of importance the study of the adsorption of polymer chains in the system with interfaces simulated by δ-functions [1] or potential wells (in some cases – by nonlinear or / and asymmetric ones). The study of the structures of such a type is also important in the theory of Bose-Einstein condensation.

In the present work, in the framework of nonlinear Schrödinger equation we study analytically the exact solutions for the problem of adsorption of real polymer chains in the system with two interfaces simulated by potential wells in the cases of both linear and nonlinear media in the wells, as well as their linear and nonlinear environment. All the possible solutions in such a system are found and the character of localization of polymer chains is studied at the conditions of continuity of the solution and its first derivative at the boundaries of the potential wells and the environment. The dependences for chemical potential for all types of possible localized states are obtained.

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PROTOTYPE OF A TENSORESISTOR BASED ON NANOCOMPOSITE LAYERS

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In medical practice, it is often necessary to control motion of various body parts (e.g., joints and chest), edema, tumors, emotions, bone tissue deformation during the post-procedure recovery, etc. For this purpose, it is convenient to use strain sensors, i.e., traditional tensoresistor gages based on metal or semiconductor materials. The tensoresistor sensors in the form of a meander made of metal foil have the low temperature resistance coefficient ($\alpha \leq 10^{-5}$ K^{-1}) and wide relative strain range ($\varepsilon = \pm 5$ %), but low strain sensitivity ($S \leq 10$), while semiconductor tensoresistor sensors exhibit the high temperature resistance coefficient ($\alpha \geq 10^{-3}$ K^{-1}), very low relative strain ($\varepsilon \leq 0.2$ %), and high strain sensitivity ($S \sim 100 - 200$) [1]. The tensoresistors of both types are difficult to bend and, therefore, limit motion of a biological object. Obviously, the efficiency of a tensoresistor can be enhanced via increasing the S and ε values and decreasing the α value. However, in traditional tensoresistors it is impossible. In view of this, we studied the temperature and mechanical properties of the layers of different nanocomposites containing single-walled carbon nanotubes (SWCNTs) in terms of their possible use as prototype of tensoresistors. The nanocomposites were prepared using different matrices (acrylic paint (AP), bovine serum albumin (BSA), or microcrystal cellulose (MCC)) filled with SWCNTs. The matrix and filler were diluted in distilled water to obtain water dispersions of groups AP / SWCNT, BSA / SWCNT, and MCC / SWCNT with an SWCNT concentration of 3 mass. %. The dispersions were used to deposit the layers by silk screening onto polyester, cotton, and office paper substrates. The resistive strain sensor prototypes were layers with a length of 15 – 20 mm, a width of 8 – 10 mm, and a thickness of 0.5 – 5 μm.

Strain studies were carried out on an automated facility, which allowed controlling the tensoresistor bending angle θ, resistance, temperature, and number of measuring cycles. The bending angle varied within ± 160 ° with a pitch of 2 °. At $\theta = 0$, the resistive tensoresistor was in the initial (unstrained) position. The dependences of resistance R on angle θ were similar for all layers: when the resistive tensoresistor was bent so as to the layers on the substrate approached one another, the resistance decreased; when the layers moved apart one another, the R value increased. At angles of ± 30 °, the $R(\theta)$ curves represented approximately linear dependences (with an error of ≤10%); beyond this range, the dependences became nonlinear. Using the minimum bending radius (~ 5 mm) and $d \leq 1$ μm, we obtained the estimate $S \sim 150 - 300$, which is of the same order of magnitude as the available data or exceeds them. The smallest value ($\alpha \sim 4 \cdot 10^{-4}$ K^{-1}) was obtained for groups BSA / SWCNT; the highest stability of the S value against moist medium was obtained for group AP / SWCNT. The high strain sensitivity ($S \sim 300$) was detected for group MCC / SWCNT.

Thus, the investigated nanocomposite layers prototype as a tensoresistor of groups AP / SWCNT, BSA / SWCNT and MCC / SWCNT are promising for use as strain and pressure sensors.

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EFFECT OF THE NANOCOMPOSITE SOLDER WITH A DYE ON THE STRENGTH OF LASER WELDS OF BIOLOGICAL TISSUES

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The broken structure and functioning of a tendon can be recovered by laser welding of broken tendon fibers with the minimum sclerostenosis [1]. At the correctly chosen parameters (wavelength, power, length, and spatial radiation profile) of the laser used and composition of a biological solder for laser welding, the tendons can be connected with an acceptable strength. Indeed, the composite solder containing nanoparticles in the form of carbon nanotubes (CNTs) in a protein matrix allows laser welds to be significantly strengthened [2, 3]. The laser weld quality can be additionally improved by introducing a small amount of a dye in the solder [4]. The advantage of such a solder is that laser radiation is effectively absorbed by the solder and actively heated. This effect makes it possible to reduce the laser radiation intensity and avoid overheating and tissue necrosis; it enhances the breaking strength and weakens the laser weld area sclerostenosis.

The strength of bovine tendon sutures was investigated using a model apparatus for laser welding of biological tissues. The apparatus generated radiation with a wavelength of 808 nm and a power of up to 8.5 W and allowed visualizing and monitoring the laser welding process. The biological tissue used was a water dispersion of the bovine serum albumin (BSA, 25 mass %) matrix, different carbon nanotube fillers (CNTs, 0.1 mass %), and indocyanine green (ICG) medical dye (0.01 mass %). The dye served as a strong absorber of laser radiation in nanocomposite solders based on multi-walled CNTs (MWCNTs), single-walled CNTs (SWCNTs), and BSA and enhanced the strength of bovine tendon laser welds. The highest breaking strength (~ 0.82 MPa) was attained for the laser welds formed with the use of the BSA / MWCNT / ICG solder. The strength of welds based on the BSA solder obtained on the references samples was < 0.1 MPa.

X-ray microtomography study of the laser weld structure showed the straight boundaries of the welds and uniformity of tendon connection over the depth and length during the nanocomposite formation between two biological tissue fragments. This is apparently due to the low probability of sclerostenosis of the laser welds.

The biocompatibility of the composite formed on the basis of both CNT types (MWCNTs and SWCNTs) in the laser weld area by growing fibroblast connective tissue cells on its surface was demonstrated.

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THE STUDY OF THE CONNECTION OF THE BONE TISSUE AND SYNTHETIC LIGAMENTS

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The existing methods of synthetic joint ligaments fixation in bone canal are imperfect (filaments, shafts, screws, etc). Sealed and less traumatic tissue connection can be obtained through the use of medical adhesives. However, “Sulfacrylate”, “Tissucol” and “LTK”, the most commonly used adhesives in medicine practice, have acrylic acids, therefore can cause allergic reactions and inflammations and do not provide high strength of connection (≤ 0.2 MPa). Strength of glued seam is several times weaker, compared with the strength of the joints obtained with sutures.

With the method of laser welding it is possible to obtain strong joints of the skin, cartilage and other tissues. High strength of the laser weld is achieved with the use of laser solder based on biocompatible nanomaterial containing the albumin protein and carbon nanotubes [1].

In this work, the nanomaterial was used in the form of a layer deposited on the synthetic ligament of the joint to its further connection with the bone channel.

Laser solder in the form of an aqueous dispersion of bovine serum albumin (BSA) and single-walled carbon nanotubes (SWCNT) were made by known methods described in detail in [2, 3]. The dispersion contained 20 wt. % BSA, and 0.1 wt. % SWCNT.

Method of silk-screen process dispersion was applied on the entire surface of the synthetic ligament, which is a weave of polyethylene terephthalate fibers by layer thickness in the range 0.2 – 40 μm. The control samples were the layers deposited on the solid substrate of the same synthetic material. Layers in liquid state were processed by laser radiation until they are completely dry. This process is similar to laser welding of biological tissues, when the dispersion of BSA / SWCNT acts as a laser solder. The parameters of used laser radiation were as follows: generation length 810 nm, power density of radiation 0.05 MW / m^2, mode – uninterrupted.

It was found that thin layers with a thickness of ≤ 5 μm have good adhesion, and thick layers (≥ 7 – 8 μm) exfoliate from the surface of the synthetic ligaments of the joints and rigid substrates. Studies of tensile strength of synthetic ligaments of the joints with layers of BSA / SWCNT nanomaterial have shown values of 10 – 15 % higher than net cords. The microhardness of the layers (thickness ≤ 5 μm) on solid substrates has reached 250 – 400 MPa, which is of the order of hardness of the natural bone tissue [4]. Preliminary experiments in vitro and in vivo have shown a positive effect of the connection by laser welding of bone tissue or synthetic ligament with a layer of BSA / SWCNT nanomaterial. Consequently, the described approach is very promising for the connection of bone and synthetic ligaments in arthroscopic plastics of the joints.

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THE MECHANISM OF LONG-RANGE INTERACTION WITH EXTERNAL IMPACT

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It is known that during ion-beam doping of semiconductor wafers defects are formed not only near surface region of the irradiated surface but also at the opposite surface, i.e. at the distance by orders of magnitude greater than the penetration depth of impinging ions. And under the influence of fast electrons in the near-surface region of opposite surface, the concentration of defects is greater than in the irradiated surface region. These phenomena are called long-range interaction effect, mechanism of which is not clear.

We propose a new mechanism for this effect based on new ideas about the movement of atoms in a substance proposed in the new molecular potential theory (MPT) [1, 2]. Unlike traditional molecular-kinetic theory the movement of atoms in a substance occurs not by overcoming the potential barrier. In MPT, the potential barrier reduces due to the occurrence of a given atom antibonding electrons and holes (antibonding quasi particles – AQPs), which at a their diffusion lengths weaken the chemical bonds of the atoms and facilitate their movement, i.e. movement of subatoms and vacancies formed by irradiation. In this way they reach the opposite surface forming a path of more complex defects. The fact that at the irradiation by fast electrons, in the surface region of the rear side the defect density is more than at irradiated surface due to the fact that the movement of created by the irradiation subatoms and vacancies requires the smaller amount of AQPs than for the destruction (recombination, when they created more complex defectsz0. Since with increasing distance from the irradiated surface concentration of AQPs is reduced, the balance of their creation process–recombination of defects is shifted towards the creation and therefore on the rear side the concentration of defects is larger.

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ON THE PHYSICAL NATURE OF THE LONG-RANGE INTERACTION THROUGH THE BOUNDARY NANOMETRY LAYER

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The atoms on the surface of the crystalline substance, which is covered with an intermediate amorphous layer of a dielectric or metal (thickness up to 30 nm) repeat the crystal structure of the base material. With increasing thickness of the intermediate layer, the effect disappears at different thicknesses depending on the properties of substances together with crystal surface and the intermediate layer. We propose a possible mechanism of this phenomenon based on a modified understanding of the nature of the chemical bond.

In contrast to the widely common idea that electrons carrying a chemical bond between two atoms are localized between them, it assumes that the density of the negative charge is distributed (with decreasing density) at large interatomic distances (the spreading of density of the negative charge occurs in the inductive and maso effects). The value of this distance depends on the average binding energy of a valence electron with the ionic core in the base material. It is determined by the ionization potentials experimentally obtained by ionization of valence electrons from the neutral atoms, but not as a result of the gradual ionization. In crystalline solids the density of the negative charge is distributed in certain crystalline directions. These density of the negative charge penetrates the intermediate amorphous layer, creating on its surface the same pattern, but not the same density that exists on the parallel cut-in layers of crystalline substances, pattern of which is applied to atoms on the surface of the intermediate amorphous layer creating a crystal lattice of the basic substance. With increasing thickness of the intermediate layer penetrating electron density gradually decreases and at a certain thickness the effect disappears.

CHARACTERIZATION OF ENGINEERED NANOPARTICLES IN SIMULATED ENVIRONMENTAL AND BIOLOGICAL SOLUTIONS

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Although, numerous research papers prove high nanoparticles (NPs) toxicity, there is still lack of information about physicochemical behavior and fate of NPs in liquid biological and environmental media. This does not so far allow predicting the behavior of engineered NPs and establish regular correlations between concentration/dose of engineered NPs and their cytotoxic effects / response.

NPs radically change their properties when entering the environment NPs due to surrounding composition and properties [1]. That is why, the analysis of nanomaterials in different matrixes should not be limited to the determination of the composition and concentration since their environmental fate is affected by particle number, charge, size and size distribution, surface area, structure and shape, state of aggregation and elemental composition. Nevertheless, the information about physicochemical behavior and fate of nanoparticles in liquid biological and environmental media (saliva, sweat, lung fluid, etc.) is still limited. This does not so far allow predicting the behavior of nanoparticles and establish regular correlations between the physicochemical state of engineered nanoparticles and cytotoxic effects.

In this work we examined how abiotic factors such as ultra-sonication, NPsloading, pH, salinity, temperature, influenced physicochemical state (particle size distribution, average diameter, surface charge, dissolution degree) of engineered NPs in simulated environmental solutions (surface water, PBS, HEPES, MOPS, Hewitt solution), biological media (saliva, lysosomal liquid), and water.

The presentation will include experimental data obtained on differently concentrated engineered Ni nanopowder produced by Advanced Powder Tech. Co (Russia). With the help of different approaches (dilution, centrifugation, filtration, sonication, etc.) we used ten-fold dilution to prepare differently concentrated suspensions of Ni NPs. Meaning thatparticles size analysisof differently loaded suspensions cannot be done with the same technique [2] we usedsingle particle inductively coupled plasma mass spectrometry (particle loading 0.02 mg / L), photon cross-correlation spectroscopy (0.2 mg / L), nanoparticle tracking analysis (2 mg / L), dynamic light scattering (20 mg / L) and laser diffraction method(200 mg/L) to quantify NPs suspensions.

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MODIFICATION OF TUNGSTEN SURFACE BY ION IMPLANTATION TECHNOLOGY

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The strength and wear resistance of nanosized surface layers of boron and carbon ion implanted tungsten have been studied. Tungsten of 99.99 at. % purity obtained by zone melting was used as initial material.

Polished plane-parallel plates with 1.5 mm thickness, 20 mm diameter and 5 – 6 nm roughness have been fabricated for ion implantation. For selecting implantation conditions bombarding ions range, displaced atoms and vacancies' spatial distribution parameters have been calculated.

Calculations have been conducted by SRIM 2013 program. Interaction of accelerated ions with target atoms is discussed in binary collision model. Tungsten samples have been implanted sequentially by boron and carbon ions with energies of 60 keV and fluencies of $\Phi = 1 \cdot 10^{16}$, $1 \cdot 10^{17}$, $3 \cdot 10^{17}$ ion $\cdot$ cm^{-2} at room temperature. Hardness testing of samples has been conducted by nano-micro indentation method. Measurements of nano-microhardness and elastic modulus have been carries out on Nano Indenter G200 (MTS Nano Instruments, USA) and Shimadzu Dynamic Ultra Micro Hardness Tester DUH-211S. Indentation on Berkovich diamond pyramid has been conducted at load-unload mode for different loads and at constant velocity of deformation. Dry friction abrasive resistance method has been used for investigating wear resistance. Three-component modified nano-sized superficial layers materials have been obtained by consistent ion irradiation. As a result new construction materials have been obtained with improved hardness (2.3 – 4.2 times) and wear resistance (3.5 – 6.3 times). Influence of ongoing radiation processes and nano-effects on mechanical properties of materials are discussed in various capability models of defects generation and target containing changes, by bombarding ions. Created modern ionimplanted construction materials are possible to apply in processing, mechanical engineering, chemical, medical and other fields of industry. The experimental results show, that high-fluencies boron and carbon ions consistent implantation represents effective method for improving hardness and wear resistance of tungsten.

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PURPLE OF CASSIUS: NANO GOLD OR COLLOIDAL GOLD?

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In the 1650's Andreas Cassius a chemist in Hamburg, Germany discovered a pigment that can be used in giving glass and porcelain a purple colour. It was prepared by adding a solution of stannous chloride to a dilute gold chloride solution. The precipitate was known as Purple of Cassius and was applied in the most famous glass and porcelain factories of Europe in Meissen in Saxony and in Sèvre in France (**Figure 1**). There were two Andreas Cassius: the father (1605 – 1673) and the son (1645 – *ca.* 1700). It is quite possible that the elder did devise a process for making the purple precipitate and it was his son who wrote *De Auro* in which he described the procedure but made no mention of his father in the book.

Figure 1. Museum pieces of glass
coloured with Purple of Cassius

Richard Zsigmondy (1865 – 1929) a Hungarian chemist in the Austrian Empire who had joined the Schott Glassworks in Jena in Germany in 1897 developed the ultramicroscope for the examination of colloids. He showed that the *Purple of Cassius* consisted of very finely divided gold with stannic oxide. For this investigation, he was awarded the Nobel Prize in Chemistry in 1925.

CHARACTERIZATION OF BORON NITRIDE COATINGS

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In this study, boron nitride (BN) is coated by physical vapor deposition – magnetron sputtering techniques. Coatings are applied on substrates by using the single crystal grown hexagonal boron nitride (h-BN) target plate. D2 steel is used for the characterizations as a substrate material. During this study the effects of the BN coating by using various coating parameters are investigated.

The thickness of the resulting coatings, nanohardness, friction coefficient, wear resistance are experimentally measured for mechanical properties. In addition, Fourier Transform Infrared Spectroscopy for crystal structure analysis (FTIR) technique is used to identify the crystal structure of BN films.

As a result of coating with different parameters, various different BN allotropes apart from h-BN are obtained. These allotropes are c-BN, w-BN, r-BN, t-BN, e-BN, and a-BN.

Correlations between coating parameters and coating properties are discussed.

THE STUDY OF MAGNETIC FIELD SENSOR OF HIGH TEMPERATURE SUPERCONDUCTING CERAMICS

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Ceramic high-temperature superconducting (HTSC) material consists of numerous granules, and Josephson transitions are formedbetween the borders. The nonlinear magnetic susceptibility of the Josephson medium is the core basis of magnetosensitive sensors. The magnetic sensitivity of weak magnetic fields (≤ 1 nT) magnet-modulation sensor (MMS) based on HTSC ceramic material of the composition (Bi–2223) is studied.

Magnetosensitive elements in the form of cylindrical rods were prepared from the prepared powder of Bi–2223 HTSC material according to well-known ceramic technology [1]. The rods had a length ~ 18 – 20 mm, diameter ~ 4 mm, the density of the critical current ≤ 10 A / cm^2, the critical temperature of ~ 103 K. Two coils were tightly wound at 16 mm of its length: the exciting one, consisting of two identical counter switched sections of 200 turns each, and on top of it – a signal one that contains 400 turns.MMS magnetosensitivity was defined as $S_U = dU/dB_0$, where U is the magnitude of the signal on the 2nd and 4th harmonics, B_0 is the measured DC magnetic field. The measurements were performed at temperature 77 K, similar to the method described in [2].

The response dependences of the second and fourth harmonics from a DC external magnetic field B_0 were recorded at different frequency f_{ac} and amplitude (peak-to-peak) modulation of the B_{ac} exciting AC magnetic field. S_U significantly increased with the growth of f_{ac} and B_{ac}. For example, the S_U magnitude ~ 500 V / T in the mode of the second harmonic, with the maximum values of f_{ac} = 50 kHz and B_{ac} = 1500 μT was much higher than S_U under f_{ac} = 20 kHz and B_{ac} = 600 μT. The sensitivity of MMS in the modes on the 2-nd and 4-th harmonics practically matched in the field of B_0 = ± 150 μT, but under the bigger fields the value of $S_U$on the 4th harmonic sharply decreased to zero and at B_0 = ± 200 μT the sign was changed.

A similar behavior of the MMS was observed at the 2nd harmonic at B_0 ≥ ± 1000 μT.
The resolution on magnetic field, magnetic flux and the dynamic range of the measurements evaluation gave values of ~ 0.2 nT, ~ 1 ϕ_0 (the magnetic flux quantum) and ≥ 120 dB, respectively. Thus, the studied MMS has the characteristics that are not practically inferior to the characteristics of the MMS based on Y–123. Moreover, it has a number of benefits: Bi–2223 ceramic HTSC material is resistant to degradation and cheaper than Y-123 ceramic HTSC. With a further selection of properties of Bi–2223 HTSC material, shapes and sizes of rods, modes and other settings, there are possible improvements of the characteristics of MMS more than 1– 2 times, thus they will be in demand in medical diagnostics (magnetocardiography, measurement of blood flow velocity), noninvasive monitoring of implanted items (stimulants, artificial heart machines, etc.), and in other applications for detection of ultraweak magnetic fields ≤ 1 pT.

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INCREASING THE CONDUCTIVITY OF LAYERS OF NANOMATERIALS BY LASER IRRADIATION

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We were studying to investigate flexible layers of the nanomatetial consisting of the acrylic paint (AP) matrix filled with multiwall carbon nanotubes (MWCNTs) and to establish the possibility of stimulation increasing the conductivity of these layers by the laser irradiation (LI).

The electrodes were formed on cotton cloth (CC). The dispersion containing AP, AP solvent (APS), and MWCNTs was thoroughly mixed with a magnetic stirrer for 24 h and then dispersed in a sonicator for 30 min. The suspension consisted of ~ 50 wt. % of the AP, 47 wt. % of the APS, and 3 wt. % of MWCNTs. The suspension was deposited onto the substrates by silk screening and dried under normal conditions. The investigated samples were divided in three groups: AP (I), AP / MWCNTs (II), and AP / APS / MWCNTs (III). Each sample was a rectangular stripe with an area of 10×20 mm^2 and a thickness of 5 – 50 μm. A half of the sample (10×10 mm^2) in the liquid state was exposed to LI with a power of 0.1 MW / m^2 and a generation wavelength of 970 nm in a continuous mode.

After multiple immersions of the samples of all the three groups in water and subsequent drying, their mass loss was controlled. The samples were kept in water for 72 h and then pulled out. The process was repeated for several times. The resulting immersion time was ~ 220 h. After the third iteration, the sample mass loss was 2 % for group I and 1.6 % for groups II and III.

The measured resistivity data were used to calculate specific conductivity σ of the samples. The obtained values are $\sigma << 10^{-7}$ S / m (group I), $\sigma \sim 10$ S / m (group II), and $\sigma \sim 10^{-4} - 10^{-2}$ S / m (group III). The σ for the samples of groups II and III exposed to LI were found to be higher than for the unirradiated samples by a factor of 6 – 8. The σ of the samples o group I did not change under LI; the LI did not affect the conductivity of dried layers either.

In the samples formed under LI or without it, heat treatment significantly increased the σ value. Upon heat treatment at a temperature of 190 °C for 30 min, the conductivity values were found to be $\sigma \sim 200 - 1000$ S / m for group II and $\sigma \sim 100 - 500$ S / m for group III. In the samples of group I, no variations in the σ value were observed.

Thus, the investigated layers consisting of the nanomaterial from the acrylic paint and carbon nanotubes are characterized by the high stability against water upon exposure for over 200 h and high conductivity (100 – 1000 S /m). These parameters make the investigated layers promising for application in biomedical electrodes and wearable electronic devices [1].

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SUPERCONDUCTING THIN-FILM MAGNETIC FIELD CONCENTRATOR WITH NANOSISED CUTS

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Optimal nanostructuring of the active strip (AS) of a magnetic field concentrator (MFC) based on superconducting films makes it possible to additionally enhance the concentration factor [1]. We calculated concentration factors F and F_0 for the nanostructured AS with nanosized cuts and for the AS without nanostructuring. In the calculation, we took into account inductances of MFC receiving rings.

The positions of cuts in the AS, magnetosensitive element (MSE) width w_0, and London penetration depth λ were varied. The MSE was placed between two MFC rings, which lied in one plane and did not intersect. In the calculations, we assumed that the cut width w_p coincides with the gap w_a between the near MFC and MSE edges and the AS width w_s and AS branch width are multiple to w_a.

The following parameters were used in the calculations: w_0 = 0.2, 1, and 5 μm; λ = 50 and 250 nm; $J_c = 10^{10}$ A / m^2 – density of critical currents; the AS hickness in the MSE 20 nm; w_s = 30 μm; ring radius r_L = 1 mm; ring width w_L = 0.8 mm; and $w_a = w_p$ = 20 nm. It can be seen that with a decrease in w_0 the F_0 value increases and the F value decreases, but the total concentration factor $F^* = F_0 \cdot F$ grows. The MFC made of low-temperature superconducting materials, e.g., niobium with λ = 50 nm, has the higher efficiency than the MFC made of high-temperature superconducting materials, e.g., Y–123 and Bi–2223 with $\lambda \geq$ 250 nm. For sample: λ = 50 nm, w_0 = 200 nm – $F^* \sim 1800$; λ = 250 nm, w_0 = 200 nm – $F^* \sim 1000$.

The investigated MFC with nanosized cuts will make it possible to enhance the efficiency of combined magnetic field sensors, superconducting quantum interferometer devices (SQUIDs), and other sensors with a resolution of ≤ 1 pT.

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CHARGE-COUPLING EFFECTS IN Si FIELD-EFFECT NANO-TRANSISTORS WITH MISIM CONTROL SYSTEM AND IN FIELD-EFFECT HALL ELEMENTS

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At present time Si nano-transistors and other Si nano-devices are produced on the base of silicon – on – insulator (SOI) structures in which thin Si nano-layers are separated from substrate by insulating SiO_2 layers. SiO_2 layers and Si substrate can represent a field element to control the operating current in Si layer. According to that, SOI nano-transistors can have system of two controlling gates (2g) represented by metal – insulator – Si – insulator – metal (MISIM) structure.

In this report will be demonstrated that varying of gate potentials of 2G transistors is accompanied by so-called charge coupling-effect (i.e. influence variations of gate potentials on transistor's channel current and on the other electrical properties. In particular charge coupling-effect changes the transistor's threshold voltage. The computer modeling and experiments with 2G transistors with different channel thickness (from 30 to 200 nm) demonstrated that quantum confinement could be allowed for transistors with a lot more Si channel thickness than theory predicts.

The charge coupling-effect also changes the electron mobility in Si layers. So by combining SOI 2G transistors and conventional Hall elements it is possible to form field-effect controlled nano-magnetosensor with high magnetosensitivity.

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NITROGEN-RICH NANOPOROUS CARBON CATALYST FOR ETHYL PYRUVATE SYNTHESIS AS A WEAPON AGAINST MOSQUITO-BORNE DENGUE FEVER

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Porous carbon materials prepared by activation of chitin and chitosan have exceptionally high concentration of nitrogenated functionalities and a typical amount of oxygenated surface groups [1]. The nitrogen content and nitrogen-containing surface species were determined by means of XPS and combustion elemental analysis. The nitrogen content was placed in the range of 2.4 – 13.1 wt. %. Dominant groups have significant basicity [2]. This material does not contain any additives such astransition metals and their oxides. Production of such carbonaceous materials is ecological because it uses natural and renewable cheap resources.

This nitrogen-rich nanoporous carbon is a selective catalyst for dehydrogenation of ethyllactate to ethylpyruvate. In turn, it appeared that precisely this compound ethylpyruvate fights mosquitoes [3] and is a chance to overcome dangerous dengue fever, a mosquito-borne tropical disease caused by the dengue virus. There are relatively few publications on the synthesis of ethyl pyruvate from ethyl lactate and the processes during the synthesis are complex, involving oxygen or other media [4]. Ethyllactate belongs to the green chemicals.

The former concept that carbonaceous surface scan catalyze dehydrogenation, e.g. of ethylbenzene [5], is still valid. New technologies open new perspectives for metal-free nanoporous carbons as catalysts for other applications [6].

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TECHNOLOGY OF THERBIUM MONOTELLURIDE NANOFILMS

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Monochalcogenides of rare-earth elements have interesting magnetic, optical, thermal, mechanical and other properties [1 – 3], but not all compounds of this class are studied rather fully. TbTe belongs to such little-studied materials. The purpose of the presented work was to develop the technology of TbTe nanofilms preparation. 0.2 – 0.8 μm thick, 6 mm long and 4 mm wide TbTe 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 mm and 43 mm. Speed of a dusting of films was equal to 55 Å / s. Temperature of a substrate changed within 720 – 1150 K. As substrates we used glass–ceramic, fused silica, sappire 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 Å 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 nm, that allows to draw a conclusion that we have nano-dimensional object.

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THE ORIGINAL METHOD FOR STUDYING OPTICAL PROPERTIES OF SEMICONDUCTOR MATERIALS AND STRUCTURES AND THE SETUP “POLYCHROMATOR”

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In the development of microelectronic technologies, along with other methods of investigation of physical properties of semiconductor materials and devices created thereon, optical methods are also very important. These methods are invaluable for investigation of physical properties of optoelectronic devices and various types of electromagnetic radiation sensors. Optical methods of measurement have proved particularly effective and efficient in terms of occurrence of nanotechnological materials, since they do not require a strong impact on the material and do not entail its structural (even local) destruction, which attracts great attention to these new methods. We have created a setup “Polychromator” – a new device for studying optical properties of semiconductor materials and structures.

In this setup, by sequentially changing optical filters in the optical range of 200 – 4100 nm we single out electromagnetic radiation packets and study the photosensitivity of the structures under investigation, such as photosensors, not only at one wavelength, but within the whole spectral packet.

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

SYNTHESIS OF In_2O_3 NANOWIRES FOR GAS SENSOR APPLICATIONS

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Gas sensors based on oxide-semiconductor nanowires have been a subject of extensive research because of their potential application in detecting several inflammable, toxic and odorless gases. Among them, In_2O_3 has been found to have a pronounced sensitivity to such gases as NO_2, NH_3, O_3, Cl_2, CO, H_2, C_2H_5OH and other species. Sensing NO_2 in the atmosphere has assumed great importance because of the serious problem of atmospheric air pollution caused by car exhaust and other sources. Recent developments showed that In_2O_3 nanowires doped with different atoms exhibit superior selectivity to NO_2, H_2S and some other gases with short response and recovery times [1 – 4]. In this work we describe the low-temperature synthesis of In_2O_3 nanowires, fabrication of a simple nanowire-network based gas sensor and its application for sensing NO_2.

In_2O_3 nanowires were grown on Si substrate using the hydrazine-assisted technology developed previously [5, 6]. This technology implies the production of volatile precursors in the vapor, formed after pyrolytic decomposition of hydrazine (N_2H_4). Indium suboxides (In_2O) were found to be the only volatile species that can provide the mass transfer from In source to the cold zone, where the In_2O_3 nanowires were synthesized onto the Si substrate. At low substrate temperatures (420 – 450 °C), the tapered In_2O_3 nanowires were grown through the Vapor-Liquid-Solid mechanism using In droplet as a self-catalyst. These nanowires had a cubic structure of the bixbyite Mn_2O_3 (I) type, which belongs to the space group *Ia3* (206). At temperatures exceeding 450 °C the growth mechanism was changed to vapor–solid one and the nanowires had uniform diameters along the growth direction with average diameters of several tens of nanometers. Considering the thermochemical reactions of synthesis it was established that kinetic factors have the main influence on the process of In_2O_3 nanowire formation. Due to this fact, even in the presence of nitriding and oxidizing species the growth of less probable In_2O_3 nanowires was observed, instead of a formation of indium nitride.

The simple gas sensor was fabricated on Si + SiO_2 substrate by depositing Ti / Au interdigitated electrodes and connecting the electrodes by bridging nanowire networks, formed after drying the droplet of acetone with dissolved In_2O_3 nanowires. The fabricated gas sensor was able to detect the concentration of NO_2 molecules down to 5 ppm level at 200 °C, with quite short and stable response and recovery time.

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FeNi NANOTUBES SYNTHESIZED IN PORES OF POLYETHYLENE TEREPHTHALATE MEMBRANES FOR BIOLOGICAL APPLICATIONS

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Biomedicine needs special chemical or physical techniques to provide novel methods of treatment on the molecular and cellular-scale. Nowadays different types of metallic nanostructures (NSs), for example, nanoparticles (NPs), nanowires (NWs) or nanotubes (NTs) are considered in case of biological applications, due to their opportunities to be targeted delivery by magnetic field with drags, be detected and visualized. In our work we show the advantages of nanotubes for bioapplication on example of FeNi NTs: homogeneous magnetic field, lower specific density and larger specific surface area.

The technique of control of shape, sizes and chemical composition of NSs is shown. It allows to set physical properties of nanotubes at stage of synthesis that opens new opportunities for drug delivery. Magnetic NTs (FeNi alloys) with external diameters 110 nm and wall thicknesses 20 nm have been synthesized in pores of polyethylene terephthalate templates using scalable and cost effective electrochemical method. Formation of NT carried out in potentiostatic mode at the deposition potentials of 1.5 V. NTs have been characterized by SEM, TEM, SAED, EDA and XRD.The analysis of dependence of the magnetic (magnetic moment at different temperatures and magnetic fields) properties from the temperature of the NT was carried out.Results of characteristics of nanotubes from another materials, such as Co, Fe, Ni and FeCo alloy for drug delivery systems were made and it was found that the smallest coertitivity where in huge magnetization have FeNi NTs, that's indicate FeNi as the best compassion for drags delivery systems.

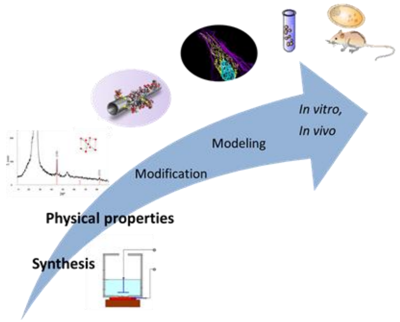

Figure 1. The main steps of verifying possibility of targeted drugs delivery by nanotubes by means of magnetic field.

The main steps of verifying possibility of targeted drugs delivery by nanotubesby means of magnetic fieldalso are consideredin our work: synthesis, characterization, investigation of physical properties, functionalized by coheres lairs, toxicity,and basic tests*in vivo* and *in vitro* must to be carried out are observed. The scheme is shown on **Figure 1**.

The step "Modification" was carried: it was obtained a reliable PMMA covering on the NT surface and bovine serum albumin was attached.

PREPARATION OF BIODEGRADABLE POLY(ESTER AMIDE) AND POLY (ESTER UREA) NANOPARTICLES BY NANOPRECIPITATION METHOD AND PRELIMINARY EVALUATION OF THEIR BIOCOMPATABILITY

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Polymeric disperse systems such as nanoparticles (NPs) and microspheres are of high interest for numerous applications in medicine, including targeted drug to a considerable potential for treatment of many human diseases. The important technological advantages of nanoparticles (NPs) usage as drug carriers are their high stability, high carrier capacity, feasibility of encapsulation of both hydrophilic or hydrophobic substances, as well as a high variety of possible administration routes, including oral application and inhalation. NPs can also be designed to allow controlled (sustained) drug release from the matrix. These properties of NPs enable improvement of drug bioavailability and might allow drug dosage decrease. The targeted and controlled administration of drugs using NPs might also help to overcome drug resistance, which is one of the major obstacles in the control of epidemics. Nanosized containers (nanocontainers) can be specially promising in ophthalmology for ocular drug delivery [1].

Various degradable and non-degradable polymers of both natural and synthetic origin have been used for NPs construction. One of the most promising for the design of NPs are amino acid-based biodegradable polymers, such as poly(ester amide)s (PEAs) and poly(ester urea)s (PEUs) which can clear from the body after the fulfillment of their function [2]. These polymers are composed of naturally occurring and non-toxic building blocks such as α-amino acids, fatty diols and dicarboxylic acids.

This research is dedicated to the systematic study of the preparation of NPs by cost-effective nanoprecipitation (polymer deposition / solvent displacement) method using PEAs and PEUs. The influence of the nature and concentration of surfactants, concentartion of polymer in the organic phase, and the ratio organic phase / inorganic (water) phase, as well as of some other factors on the size of the fabricated nanoparticles have been studied. It was established that depending on the used conditions the NPs size could be tuned within 40 – 330 nm, zeta-potential up to + 28 mV. As the next step of this research an evaluation of biocompability and bioavailability of the synthesized nanoparticles has been performed, using two stable human cell culture lines – HeLa and A549. This part of study is still in progress now.

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NANOCOMPOSITES BASED ON POLYURETHANE/POLY(2-HYDROXYETHYL METHACRYLATE) POLYMER MATRIX AND NANOFILLERS MODIFIERED BY BIOLOGICALLY ACTIVE SUBSTANCES FOR BIOMEDICAL APPLICATION

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The nanocomposites based on polyurethane (PU) and poly(2-hydroxyethyl methacrylate) (PHEMA) semi-IPN and nanofillers modified by biologicaly active substances (BAS) for future biomedical applications were created. As BAS the aminoacids – histidine, glycine, lysine and tryptophan; antiseptics – salts of silver, zinc and copper; metronidazol, decametoxine were used. The structure peculiarities, physico-mechanical properties and biocompatibility have been investigated.

The structural characteristics of the nanocomposites were obtained by small-angle X-ray scattering. It was shown that the native polymer matrix has two hierarchical levels of heterogeneity. The first one is the concentration fluctuations with size of 7.5 – 12.5 Å, and the second level of heterogeneity characterized by the release of the microinclusions almost pure polyurethane and PHEMA domains. The introduction of nanofiller fundamentally changes the nature of the scattered intensity. The diffraction maximum (polyurethane) almost completely disappears and also a maximum of semi-IPN, located at wave vector value $q^* = 0.25$ vanishes. In the case of polyurethane matrix, nanofiller at its minimum content (1 %) is uniformly distributed in the bulk material, while increasing content of densil leads to aggregation of nanofiller in the form of mass-fractal structures. Entering the second polymer component into the matrix leads to an increase in the threshold of a uniform distribution of filler in the case of semi-IPNs with PHEMA content 17% from 1% to 3%, and in the case of semi-IPNs with PHEMA content 37 % – from 1 to 5 %. Raising the threshold of homogenization of nanoparticles distribution is the result of reorganization of filled polyurethane during process of its swelling in the monomer HEMA and further photopolymerization.

Examination of antibacterial properties against a number of aerobic micro-organisms and anaerobic microorganisms was carried out and membranotropnyh properties in according to cell culture Saccharomyces cerevisiae was done. The antibacterial activity of nanocomposites against anaerobic microorganisms was found, i.e. depressing effect on the growth of bacteria.

The release of biologically active compounds from the nanocomposites into the environment was investigated and was shown that the introduction of nanofillers modifiered by monolayers and by heterolayers of BAS and variation of polymer matrix components allowed to regulate the rate of release of biologically active substances into the environment.

A study of cytotoxicity and histocompatibility of the created nanocomposites in experiments with rats were done. The blood analysis and tissue biopsies for histological studies were performed after 1 – 18 days of nanocomposites implantation. The symptoms of inflammation in the tissues surrounding implant and the violation of blood parameters of the animals were not observed.

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CONTROLLING EMISSION OF NANO-SCALE PARTICLES FROM ENGINES WITH PARTICLE-GROUPING CONCEPT

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Grouping of particles / droplets in oscillating flows has ramifications to various industrial and natural two-phase flows, such as: fuel sprays, particulate matter (PM) emitted from engines, colloids in water [1], and atmospheric aerosols. The mathematical analysis of this phenomenon leads to the prediction of grouping tendency as a function of the parameters that play a role in the process [2]. One of the applications is the design of an exhaust system for vehicle-engines (Diesel & Gasoline) that enhances particle grouping and coagulation and hence leading to the increase of particle size, while enabling efficient filtration, and to the reduction of risk associated with exposure to sub-micron and nano-scale particles [3, 4]. Brownian motion, grouping, coagulation as well as particle formation are taking place simultaneously, as a function of particle size-scale. These combined processes will be elucidated, and the mathematical model and supportive experimental results will be presented.

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PECULIARITIES OF "ALLOY" SCATTERING IN SEMICONDUCTORS

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There is investigated the effect of nanometer size disordered regions in Si_xGe_{1-x} and InP_xAs_{1-x} semiconductor alloys on the charge carriers mobility. An investigation has shown that composition dependence of the mobility appears as result of competition of main processes of current carriers scattering on phonons, ionized impurities and "alloy" disorders in Si_xGe_{1-x} and InP_xAs_{1-x} alloys. We have calculated the contribution of these scattering processes into total scattering. Share of contribution of "alloy" disorders into the total mobility is different for Si_xGe_{1-x} and InP_xAs_{1-x} solid solutions. Unlike Si_xGe_{1-x} alloys the "alloy" disorders in InP_xAs_{1-x} practically do not disturb the crystal lattice in tangible way at temperatures in the range of 4.2 – 300 K because of sublattices of InP and InAs retain a certain individuality in InP_xAs_{1-x} alloys.

NANOSIZE CLUSTERS IN COMPOUNDS InAs AND InP AND THEIR SOLID SOLUTIONS InP_xAs_{1-x}

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The compounds of indium arsenide, indium phosphide and their solid solutions are important materials for optoelectronics, microelectronics and nanotechnology. It is known that the stabilization of nanoparticles is a major problem in modern nanotechnology. The carried out investigations in presented work can give interesting information in the indicated direction. It has been shown, that it is possible to create nanoscale clusters in crystals with the help of hard radiation, wherein it is possible to manage sizes of inclusions in the range of 1 – 100 nm as well as they may be larger and smaller sizes.

Investigations of very slow diffusion processes in irradiated crystals give an opportunity to reveal abnormal behavior of nanoscale clusters. It has been shown that in certain materials the curves of the frequency dependence of the optical absorption coefficient near the fundamental edge at $T = 300$ K for a long time (two years) do not shift to the "restoration", but move to the opposite direction. There have been studied the electrical and optical properties and the heat treatment processes (annealing) of crystals irradiated with fast neutron fluxes ($\Phi = 2 \cdot 10^{18}$ n / cm^2), and high-energy electrons with $E = 50$ MeV and $\Phi = 6.0 \cdot 10^{17}$ e / cm^2. As a result, the mechanism of anomalous phenomena has been established.

It was found that nanosized clusters contribute to a significant increase in the basic parameter of the thermoelectric material- thermoelectric efficiency.

There has been established scattering mechanism of electrons on nanosized clusters.

On the other hand, the possible influence of nanoscale clusters as well as small point type defects on important parameters of the materials, in particular, the concentration, charge carriers mobility, electrons effective mass and the degree of non-parabolicity of the conduction band, and crystal lattice vibrations have been analyzed.

THE ROLE OF Fe_3O_4 NANOPARTICLES ON SUPERCONDUCTIVITY OF MgB_2

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We report the effect of electrohydraulic treated nano Fe_3O_4 doping on the superconducting properties of MgB_2 [1]. An important goal of substitution / doping is enhancement of pinning in MgB_2. In spite of impressive progress on improving the critical current density (J_c) [2] at temperatures above 20 K, which is considered to be the benchmark operating temperature for this material, $J_c$rapidly drops with increasing magnetic field (H) due to its poor pinning ability.

In general, MgB_2 has poor grain connection and a lack of pinning centers, and hence often exhibits a rapid decrease in critical current density (J_c) in high magnetic fields. Fortunately, through the formation of nanoparticle structures in bulk MgB_2 [3] and thin films, the problem of the poor grain connection can be solved, and the flux pinning force can also be significantly enhanced due to an increase of pinning centers served by grain boundaries. In order to improve the performance of MgB_2 further, it is necessary to introduce more pinning centers, especially those consisting of nano-sized second-phase inclusions, which often provide strong pinning forces. In this direction, several types of nanoparticles have also been substituted/doped in MgB_2.

We consider the effect of nano Fe_3O_4 doping on the superconducting properties of MgB_2. To do this, we for the first time turn on the electrohydraulic effect (Yutkin effect) [4] in a well-known scheme for the treatment (synthesis) of nanoparticles in order to significantly reduce departure from average size of particlesand for ensuring the reproducibility of the synthesis process of the composite MgB_2–Fe_3O_4.

Nano-Fe_3O_4 (of various sizes) doped polycrystalline MgB_2 samples were synthesized by encapsulation of well mixed high quality Mg, B and nano- Fe_3O_4 powders. In order to study the effect of magnetic particles on superconductivity, the composites of $(MgB_2)_{0.98}(Fe_3O_4)_{0.02}$ was synthesized with former sintered at different temperatures. The superconducting properties were investigated in the case of samples sintering at high temperature (750 °C) and at low temperature (350 °C). We have investigatedthe effect of the addition of several concentrations of magnetite Fe_3O_4 nanoparticles on the microstructure, critical temperature T_c and the critical current density J_c in the composite MgB_2–Fe_3O_4 material. The study was conducted using X-ray Diffraction (XRD), Energy Dispersive X-Ray Spectroscopy (EDS) and Vibrating Sample Magnetometer (VSM) for the magnetization measurements.

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CHEMICALLY TAILORED NANOSTRUCTURED SEMICONDUCTOR MATERIALS

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New selenium precursors are always difficult to synthesize and then adopt them for the nanotechnology. Simpler approaches are mandatory for making quantum dots to find commercial viability. Chemistry of CdSe magic-size and regular QDs from organo-Se-precursor using concepts of solution chemistry is an attractive option [1 – 3]. The selenadiazoles are found to be excellent precursors for preparation of quantum dots of CdSe and other metal selenides which can alter the face of nanotechnology. Applications of 1,2,3-selenadiazoles in material chemistry are mainly due to their ability to release free active Se during thermolysis or photolysis. The optical behavior of such particles is dependent on ratio of selenium and metals, e.g. with increase in particles size, the band-gap shifts to red region. The control of size and size distribution for various applications is a challenging part of such materials synthesis. However, with reasonable design and understanding of growth and nucleation mechanism these high tech tiny nano-crystals have potential to revolutionize the photonic industry. These tiny clusters emit white light when illuminated under 365 nm UV light source. Similarly, 1,2,3-selenadiazole have been successfully employed as selenium precursor in the synthesis of $CuInSe_2$ nanoparticles. Change in various reaction parameters such as reaction temperature, amount of oleic acid (OLA) and capping agents showed change in the physical characteristics of the CISe nanoparticles. The changes in the reaction parameters were resulted in change in physical appearance of CISe NPs with respect to the nanoparticle shape and size (**Figure 1**)..

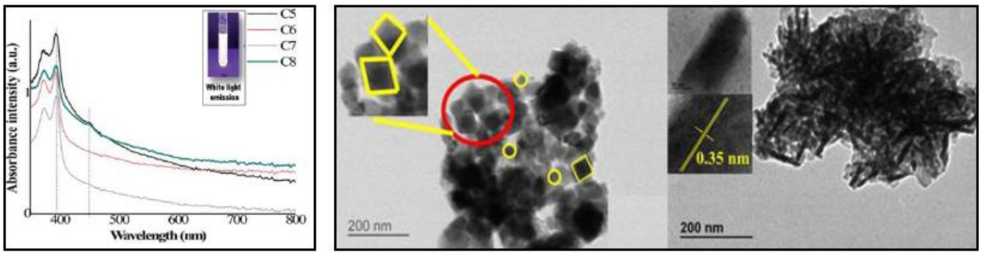

Figure 1. CdSe magic-clusters and CISe by use of 1,2,3-selenadiazoles

Degradation of various organic dyes by use of ZnO based photocatalysts employing plasmonic photocatalysis or by use of anatase and rutile TiO_2 nano-particles along size core / shell type oxide catalysyt is attractive option for dye degradation. It is observed that at certain conditions, rutile is as effective as anatase for the degradation of methylene blue dye solution. Oxygen surfaces are often advantageous. Starch coated precursor revealed formation of anatase particles even at 100 °C. Sintering up to 400 °C retained phase pure anatase crystal structure however the total conversion to rutile phase resulted after sintering to 800 °C. The photocatalyst reusing after five cycles retained the degradation efficiency of 83 % and 71 % respectively for anatase and rutile when tested for methylene blue.

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NANOTECHNOLOGY-BASED REMEDIATION OF PETROLEUM IMPURITIES FROM WATER

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The nanotechnology-based methods for removal of oil in petroleum spills and its separation from water are discussed. Oil spills during petroleum extraction and processing are frequently unavoidable and could lead to events of distinct scale, from small contaminations of ground and sea water up to huge disasters. In addition to classic methods of oil removal, the “nano”-techniques are being currently developed, which use nano zero-valent iron (nZVI), carbon nanotubes, sponges, aerogels and nanocomposites, metal and non-metal nanostructurized oxides, nitrides, salts, and zeolites. Some of these nanomaterials can be prepared by “greener” methods at lower costs and without damage for the environment. Nowadays, these methods (except nZVI) are applied still in small scale due to insufficient knowledge of their toxicity or they are subject of laboratory studies. Experimental data of remediation processes on the basis of carbon allotropes, metal oxides, xerogels, magnetic components, and organic and inorganic peroxides will be discussed in this presentation. Oil deep oxidation occurs due to free radicals appearing as a result of fenton-type reactions, and final solidification of carbon-hydrocarbon mixture takes place leaving water free of oil drops.

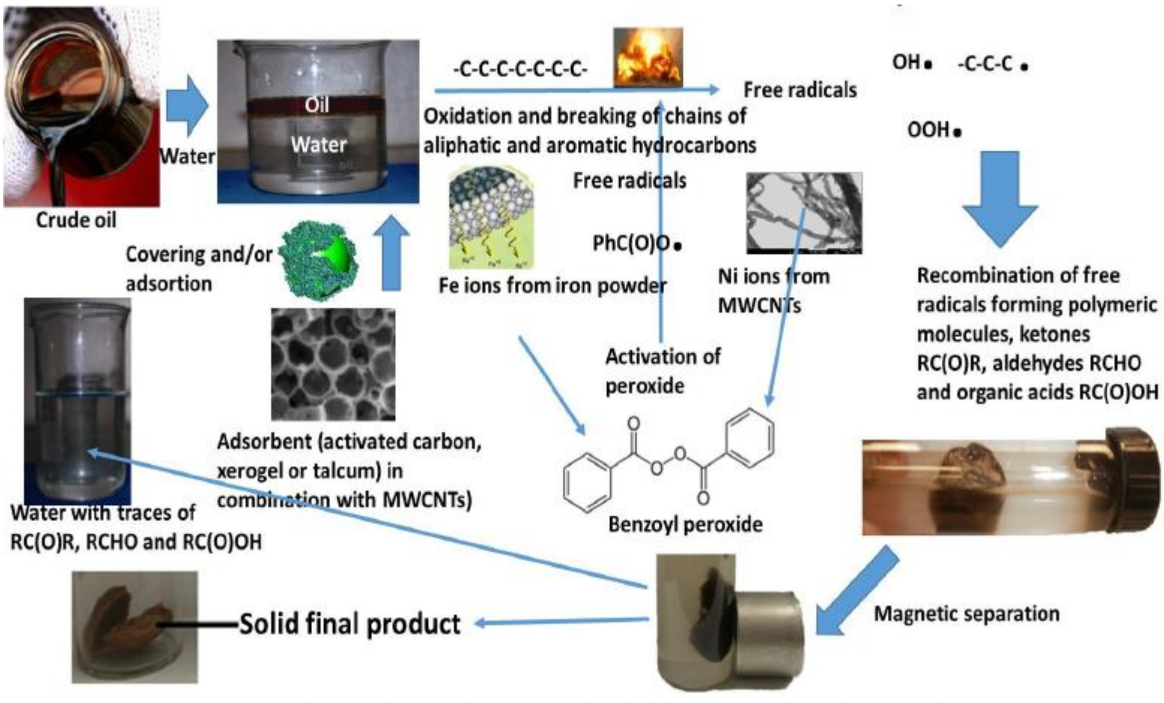

Figure 1. Scheme for oxidation and solidification of crudr petroleum.

Resulted solid phase can be easily separated from water by decantation or using a magnet. The separation efficiency in distinct systems (**Figure 1**) is in the range 92 – 100 %. Main attention is paid to simplicity and commercial availability of applied nanomaterials.

THE MAGNETIC STATES OF THE OXYGEN VACANCIES IN VICINITY OF THE OXIDE NANOSTRUCTURED SURFACE

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Nanomaterials (nanoparticle powders, nanograin ceramics and thin films) are known to be in confinement conditions defined by surface and surrounding it media. In general case, characteristics of these materials properties size effects depend on surface to volume ratio. For small enough sizes (from a few nm to several tens nm) the contribution of surface becomes dominant. Allowing for surface properties are strongly different from those in bulk we are faced with possibility to have nanomaterials with properties absent in bulk. Experimental results confirm this statement. For example, such striking phenomenon as observation of ferromagnetism at room temperature in spherical nanonparticles (size 7 – 30 nm) and thin films of nonmagnetic in bulk oxides CeO_2, Al_2O_3, ZnO, etc. has been reported respectively in [1] and in [2, 3]. The detailed theoretical explanation of these phenomena is absent up to now. The appearance of ferroelectricity in nanosized incipient ferroelectrics [4], which in bulk remain paraelectric up to zero K, as well as observed enhancement of spontaneous polarization up to chemical decomposition of Rochelle salt nanorods of 30 nm diameter[5], was explained theoretically[6] by taking into account the influence of surface and originated from it and surrounding media mechanical tensions as well as symmetry lowering in vicinity of surface. The latter was shown to be extremely important because it leads to appearance in small enough nanosystems piezoelectric, piezomagnetic and magnetoelectric properties [7], which can be absent in the bulk. Spontaneous flexoeffects absent in bulk were forecasted for nanosystems [8].

Surface induced magnetization in binary oxides and incipient ferroelectrics was considered recently [9, 10] by taking into account the lowering of the vacancies and impurities wave functions symmetry in vicinity of surface. We developed for the first time the theory of magnetization appearance in thin films of nonmagnetic in bulk binary oxides. In particular, considering in accordance with experiment [2] and theory [11] oxygen vacancies as the sources of magnetization, we explained the influence of film thickness and substrate on magnetization and appearance of hysteresis loops. We demonstrate these features by comparing the theory with experimental data obtained in SnO_2 film [11].

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ABILITY OF LUMENOPHORS TO DETECT MICROCRACKS IN METALLIC CONSTRUCTIONS

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Luminescence defectoscopy is based on the ability of a luminescent test solution (solution of luminophor in the organic solvent) to penetrate unnoticeable surface defects (1 μm) and then lighting in the UV radiation area to display their character and location.

Synthetic luminophors used in luminescent defectoscopy have high luminescent properties but at the same time are expensive and toxic.

The aim of the research is to improve worked out by us simple technology [1 – 4] to release high effective non-toxic luminophor from natural raw material and reduce it to the licensing condition.

Luminophor obtained by the offered technology has high operational properties. In particular, it has an ability to detect microcracks less than 1 μm; luminescence intensity in relation to the standard – uranil nitrate is 450 – 500 %, color factor is greenish-yellow; the product is cheap, high adhesive and stable that corresponds to the International Standards.

The suggested technology is based on the use of local inexpensive raw material. In comparison with the prototypes it excludes two power-consuming steps, therefore the technological process becomes simple and the first cost of the production lessens.

The use of the suggested lumiphor is prospective in nanomaterial techniques, biology, medicine, analytical chemistry, criminalistics, poligraphy manufacture of luminescent dye and others.

Luminophor obtained by our technology is unique due to a simple way of its reception. This way is to combine chosen purposely some oil fractions and further express distillation in deep vacuum. At the same time it does not need additional cleaning.

The mentioned luminophor is used to detect microcracks less than 1 μm in parts of a machine, metal constructions, concrete, glass, plastic, etc.

1. Method for producing oil for fluorescent inspection. USSR Inv Dipl. #246762.
2. Method for producing luminophor. Georg. Patent #P4054.
3. Penetrant – “Pentrex” (UK).
4. Penetrant – “Lg-6” – Ukraine.

LOW-FREQUENCY NOISES OF DOUBLE-GATED SiNW FET UNDER IRRADIATION

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The noise characteristics of an array of silicon nanowire p^+–p–p^+ field-effect double-gated lateral transistors are investigated. Upright (vertically) it is bioliquid–insulator–semiconductor structure. Front gate is the reference electrode located in bioliquid. Thicknesses of front and buried oxide layers are 8 and 145 nm, NW length and thickness are 20 and 250 nm, correspondingly.

Figure 1 shows the spectral dependence of the low-frequency noise for bare transistor, measured under irradiation, as well as in the dark, at 300 K.

For description of low-frequency noise we used the correlated number-mobility fluctuation unified $\Delta n - \Delta\mu$ model. According to this model, the flicker noise spectral density can be presented as follows (K. K. Hung, et al. IEEE Trans. ED, 1990, 37, 645):

$$S_{V_{DS}}(f) = \frac{e^2 kT}{\gamma f w l\, C_{ox}^2}(1 + \alpha\mu_h p)^2 N_t(E_f).$$

Here w and l are the channel width and length,respectively, C_{ox} is the capacitance of the insulator layer, $\gamma = 4\pi\sqrt{2m_{ox}^* \phi_B}/h$ is the tunneling parameter (10^8 cm^{-1}), ϕ_B is the tunneling barrier height for majority carriers at the interface, m_{ox}^* is the hole effective mass in the oxide layer, $\alpha = \pi m^* e^2/4hkT(\varepsilon_{Si} + \varepsilon_{ox})^2$ is the carrier density function formed by the screening effect, m^* is the hole effective mass in the silicon, μ_h is the hole mobility, $N_t(E_f)$ is the energetic distribution of the traps, and E_f is the Fermi energy.

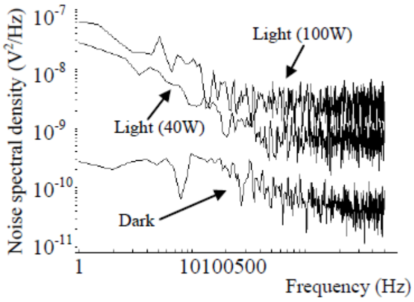

Figure 1. Spectral dependence of low-frequency noise, measured at irradiation (under of 100 and 40 W power incandescent lamp) as well as in the dark at 300 K, $V_{\mathrm{BG}} = -1$ V.

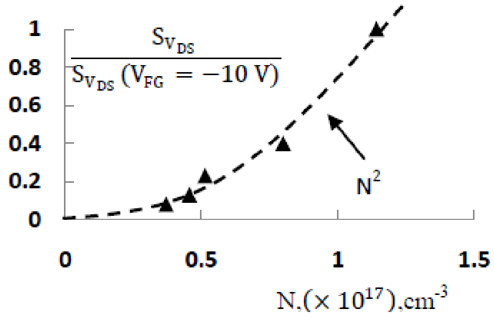

Figure 2. Normalized noise dependence vs. carrier's concentration ($f = 50$ Hz).

As follows from the abobe equation, $\propto p^2$. The curve presented in **Figure 2** provides evidence in favor of the application of the unified $\Delta n - \Delta\mu$ model to describe the noise, showing the dependence of the normalized noise vs. the concentration of the majority carriers. This is a quadratic dependence on concentration. **Figure 2** plotted using above mentionet data and $\mu_h = 125$ cm^2 / V· s.

EFFECTIVE SEGREGATION COEFFICIENT OF IMPURITIES IN Si AT PULLING FROM MG-Si MELT

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Today and in the near future Si is just one practically applied the basic active component of modern high-performance semiconductor devices. There is currently no contestant to silicon electronics technology. However, simple Si devices scaling cannot go on forever. The dimensions shrink of macro crystalline Si to the manometer range broadens the silicon range of applications. Silicon technology is gradually moving into new applications as novel silicon-base nanotechnology on the world economy. However further development of Si application requires increasing of investigations in the direction of identification of behavior uncontrolled impurities in Si. Minimization of impurities content in Si, intended for its application as semiconductor material, is realized by using many known traditional refinement methods, among them crystallization from melt. In given work directional crystallization is used for purification directly metallurgical grade Si (n-MG-Si) with 98 mass % Si purity without intermediate stages.

We have shown that after pulling from melt n-MG-Si goes into p-type Si with current carriers concentration $p \sim 10^{16}$ cm^{-3} and Si has been purified practically from majority of impurities. The possibility of uncontrolled impurities removal from Si depends on impurities effective coefficient of segragation in Si. Therefore we have investigated the effective coefficient of segregation of unwanted impurities in Si crystals, obtained by pulling directly from MG-Si melt. In the presented article the effective segregation coefficient of major impurities in Si has been calculated and analysed in the dependence on the crystallisation conditions. Effective coefficient of segregation makes possible to estimate the capacity and efficiency of Si purification from impurities during crystallization from melt.

PHOTODYNAMIC EFFECT ON DNA IN THE COMPLEX WITH INTERCALATORS

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The aim of this work is to study the interaction between laser irradiation (457 nm) and intercalators, in particular acridine dyes, acridine orange (AO) and proflavin (PF) in free condition and in the complex with DNA using methods of spectrophotometry and fluorescence.Analysis of absorbtion and fluorescence spectra shows that discoloration and destruction which happens with intercalators in free condition significantly decreases in the complex with DNA.

We proposed that in case of DNA complex with AO at photodynamic effect in solutions the principal oxidant is not an oxygen molecule but H^+ ions. It should be noted that at photodynamic effect H^+ local concentration depends on electrolytic dissociation of water molecule. So, at photon absorption by chromophore a part of energy dissipates into heat as a result of conversion which we consider as energy transfer from electron vibration levels of organic molecules to water molecule vibration levels and it should increase the constant of electrolytic dissociation. In the place where AO exited molecule undergoes total energy dissipation we can get high local concentration of H^+ and OH^- ions in immediate proximity from DNA, and thus hydrolyze possibility of both phosphordiester and glycoside linkages is significant.

DEVELOPMENT OF NANOCOMPOSITE FOR METRONOMIC PHOTODYNAMIC ANTICANCER THERAPY

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Photodynamic therapy (PDT) is comparatively innovative, minimally invasive and highly attractive modality for the tumors treatment. PDT bases on a photosensitizer, a powerful light source (laser) which wavelength matches the absorption spectrum, of the photosensitizer and oxygen. PDT is recognized as a multimodality treatment procedure [1]. It is worth noting, that metronomic PDT (mPDT), one of the PDT modifications [2], based on the techniques where both the photosensitizer and light are delivered prolonged and gradually at low rates to increase selective tumor cell kill mostly through apoptosis.

The aim of the present work is to create a new nanocomposite for the solid tumors treatment. First of all, chitosan nanoparticles were prepared using dissolved chitosan in 2.0 % (v / v) acetic acid and further sodium tripolyphosphate was dropped slowly with stirring. Chitosan nanoparticles as a suspension were collected and stored in deionized water [3]. Poloxamer 407 (Lutrol or Pluronic F127) in concentration 21 % was used for creation of stable density conditions to plyronic. Gematoporfirin was picked as a photosensitizer. Finally, to rate the velocity of gematoporfirin releasing all samples were incubated at 37 °C with sodium phosphate buffer. The concentration measurement was made by NanoDrop 1000 (“Thermo Scientific”, USA).

Based on results the developed nanocomposite can prolong gematoporfirinrelease for 8 days. As well in conclusion it should be mention that temperature-dependent properties of poloxamer 407 in concentration 21 % provide the centralization of gematoporfirin depot in the gel form nanocomposite. In the end it’s promotes target delivery.

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ELECTRICAL AND STRUCTURAL PROPERTIES OF Zn-BASED NANOPARTICLES IN SiO_2 PRODUCED BY ION-BEAM SYNTHESIS

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The paper presents electrical and structural properties of produced by ion-beam synthesis of Zn nanocrystals in SiO_2. Samples were performed by using an implantation of high dose zinc ions with energy of 130 keV and annealing process in 700 °C. Using electron microscopy was established that annealing causes extension of admixtures distribution on depth and zinc nanoparticles size increasing from 1 – 6 to 12 – 18 nm. For prepared material AC conductivity measurements were made in temperatures range from 77 to 373 K and at frequencies range from 50 Hz to 1 MHz. Strong frequency dependence on conductivity proves that in this nanocomposite Zn–SiO_2 conduction takes place by electron hopping exchange (tunneling) between metallic phase nanoparticles. It was established that three activation energies of conductivity occurs in temperatures range – in low temperatures $\Delta E_1 \approx 0.001$ eV, in medium temperatures $\Delta E_2 \approx 0.025$ eV and in higher temperatures area $\Delta E_3 \approx 0.096$ eV. This is due to the presence of at least two types of nanoparticles. First there are zinc nanoparticles with zinc oxide coating, second there are nanoparticles without the coating. The highest activation energy occurs during electrons tunneling between nanoparticles with zinc oxide coating. Intermediate activation energy corresponds to tunneling from nanoparticle with coating to nanoparticle without coating or conversely. The lowest activation energy corresponds to electrons hopping between nanoparticles without coatings.

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LUMINESCENCE OF F-CENTERS IN CeO_{2-x} NANOCRYSTALS

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CeO_{2-x} nanocrystals (nanoceria) are widely investigated nowadays due to their strong catalytic, oxygen storage and antioxidant properties determined by high oxygen capacity and easy reduction of Ce^{4+} ions to Ce^{3+} ones. These properties of nanoceria are in turn determined by both concentration and location of oxygen vacancies in ceria lattice which content can be controlled by variation of treatment atmosphere, nanocrystal size and additional doping of nanoceria by di- or trivalent cations.

Steady state and time-resolved luminescence studies enable us to distinguish two types of optical centers in ceria nanocrystals formed by Ce^{3+} ions which charge is compensated by oxygen vacancies in NN positions, and Ce^{4+}–O^{2-} charge transfer (CT) complexes, respectively. Also it was determined that ratio between intensities of Ce^{3+} $5d \rightarrow 4f$ luminescence and CT luminescence in Ce^{4+}–O^{2-} complex depended strongly both on the atmosphere of treatment [1] and size of nanocrystal [2]. Increase of the content of oxygen vacancies either due to treatment in reduction atmosphere or decrease of nanocrystal size led to corresponding increase of Ce^{3+} luminescence intensity as compared to CT band. However, presence of alternative paths of electron behavior after oxygen vacancy formation besides localization on cerium ions, such as formation of F-centers, can complicate sufficiently this rather simple picture. In this work we show that F-centers of different types are inevitably formed in ceria lattice even at treatment in oxidative atmosphere leading to rather complex pattern of CT excitation relaxation. F-centers can serve both as alternative luminescence centers, so as shallow CT excitation traps leading to a series of trapping–retrapping acts during excitation lifetime.

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SILVER NANOPARTICLES IN THE BRANCHED WATER-SOLUBLE POLYMERS DEXTRAN–POLYACRYLAMIDE MATRIX

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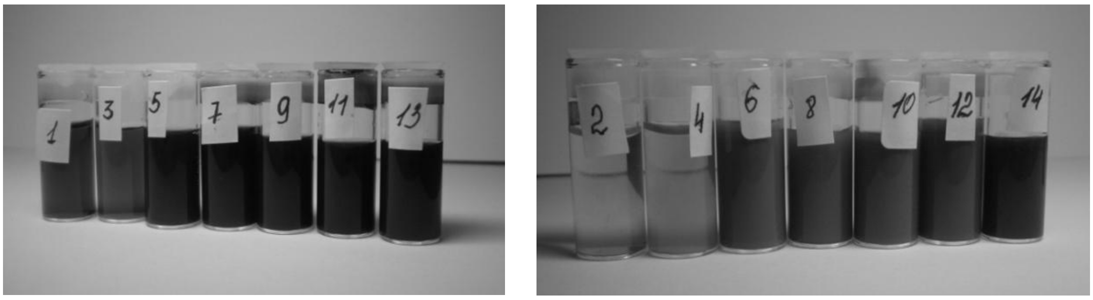
Noble metal nanoparticles are the subject of focused researches due to their unique electronic, optical, biological properties. These properties deal with small size and large specific area. For these reason metallic nanoparticles have found uses in various field as catalysis, electronics medicine, pharmacy, food manufacturing, waste-water treatment, etc. Silver nanoparticles can be used as antibacterial agent. Because of their high reactivity due to large surface to volume ratio, they can inhibit bacterial growth in aqueous and solid media.

There is an array of routes to obtain Ag colloids. Among them the chemical reduction of silver salt in polymer matrix is the most prominent technique for in situ Ag NPs synthesis. The nature of reduction agent, pH and temperature conditions, nature and structure of polymer matrix significantly affect the process of NPs formation and could control their shape, size and size distribution.

Our idea was to obtain silver nanoparticles (Ag NPs) in water soluble polymer matrices of various molecular structures. We used linear Polyacrylamide (PAA) and branched copolymers Dextran-g-Polyacrylamide in nonionic and anionic forms (**Figure 1**). The action of reducing agents (sodium borohydride, sodium citrate or hydrogen) and the influence of temperature of reaction were investigated. The nanosystems were characterized by UV–Vis spectroscopy, TEM microscopy, small-angle X-Ray, dynamic light scattering.



a **b**

Figure 1. Ag NPs synthesized in nonionic (a) and anionic (b) linear (1 – 4) and branched (5 – 14) polymer matrices.

It was found out that PAA and synthesized copolymers in solution affected the process of Ag NPs formation at different temperatures. The template role of the host polymer for the *in situ* synthesis of nanoparticles consists in improvement of the nanoparticle dispersion inside the polymer matrix and also in prevention of the aggregate formation. Branched polymer matrices allow obtaining stable silver colloids even at high temperature when the linear PAA matrix is not efficient.

This investigation was supported by NATO Grant CB.NUKR.CLG 98424.

SILICA-COATED MAGNETITE AND COBALT FERRITE NANOPARTICLES: SYNTHESIS, FUNCTIONALIZATION, MAGNETIC PROPERTIES AND APPLICATIONS FOR OPTICAL SENSING

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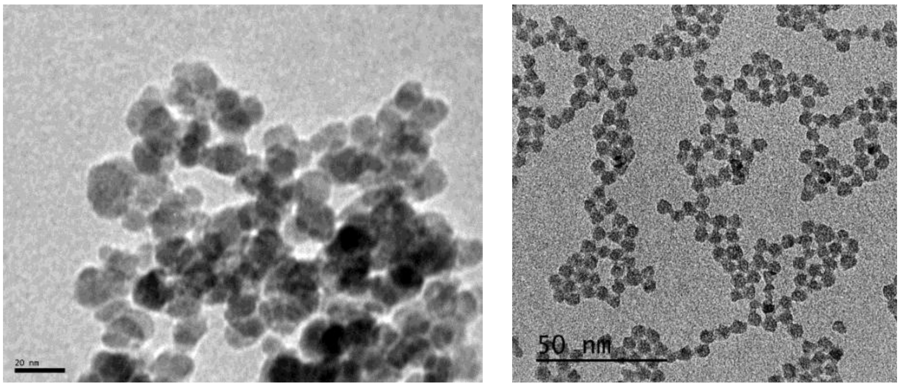
Magnetic nanoparticles with spinel structure MFe_2O_4 (M = Fe, Co, Mn, Ni, Cu, Zn, etc.) have many important applications especially in engineering nanodevices, in the biomedical industry, and also useful for environmental processes. Among the new explored magnetic particles magnetite (Fe_3O_4) and cobalt ferrite ($CoFe_2O_4$) has one of the most potential. It is important for all these technologies and applications to produce superparamagnetic nanoparticles (with diameter less than 10 nm), a narrow size distribution, pure and stability a long time. The physical and chemical properties of magnetite nanocrystals are greatly affected by the synthesis route, and for this reason various approaches have been employed to produce magnetite in order to obtain expected properties.

In this work, we reportpreparation of magnetic nanoparticles of cobalt ferrite have been synthesized by wet chemical method using stable ferric and cobalt salts in the basic medium. X-ray Diffraction (XRD) and Transmission Electron Microscope (TEM) confirmed the formation of single phase cobalt ferrite and magnetite nanoparticles in the range 5 – 10 nm depending on the annealing temperature and time (**Figure 1**). The size of the particles increases with annealing temperature and time while the coercively goes through a maximum, peaking at around 28 nm. A very large coercivity (90.5 kOe)is observed on cooling down to 77 K while typical blocking effects are observed below about 260 K.



a **b**

Figure 1. Comparative TEM images of magnetite (a) and cobalt ferrite (b) particles prepared by co-precipitation method.

One of them the most popular rout is based on the covered Fe_3O_4 with a chemically inert a think silica layer consist amino or other functional organic groups. FTIR spectra core–shall nanoparticles of $CoFe_2O_4$ and Fe_3O_4 has Si–O–Si bond's stretching at 1080 and 800 cm^{-1}, which indicates that the silica has successfully coated surface of nanocrystallites. The magnetic dipole attraction decreases quickly with the increase of size of particles and thickness of silica shell. The using of sulfonate polyelectrolytes allows to obtained core-shell particles with ion-exchange properties. These particles modified with ion Eu(III) was used for development of optical sensors for antibiotics determination.

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USING NANOPARTICLES FOR MODIFICATION STRUCTURE OF WELD METAL HSLA STEELS

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Currently, the main control method of the crystallization of the liquid metal in metallurgy and welding is: the introduction of foreign particles into the melt modifiers, nucleating future; the use of additives (surfactants) which are adsorbed on the surface of the nuclei and reduce the surface tension at the interface of the growing crystal from the melt; use of an external mechanical or electromagnetic effects.

Experimental data show that the most promising way to increase the properties of weld metal of high alloy steels is the use of exogenous refractory particles of different compounds (oxides, nitrides, carbides, borides) nano-sized (≤ 100 nm) range.

The results of studies of the structure of high-strength low-alloy weld metal steel 14HGNDTS modified nanopowder particles of various refractory compounds – nitrides, carbides and oxides of various metals (TiC, TiN, SiC, VC, NbC, TiO_2, Al_2O_3, MgO, ZrO_2). The particles are introduced into the composition of the required core cored wires that were used in automatic arc welding under a layer of activating ceramic flux.

A feature of using welding to modify the structure of the weld metal is a need to protect the input of powders from the direct effects of the arc to prevent complete melting or evaporation. Therefore, the introduction of the technology used in the flux-cored wires on the "cold" part of the weld pool with a temperature of about 1600 – 1800 °C.

The paper studied the structure of the modified weld metal, set the distribution pattern of nanoparticles and to determine their impact on the formation of the structures of the needle, polygonal ferrite, bainite. It was built CTT diagrams decomposition of austenite, the temperatures of phase transformations and calculate the total number of formed phases.

It is found that the use of nanoparticles carbide VC, NbC or SiC for the modification of weld metal leads to the formation of predominantly bainitic or bainite–martensite structures (from 40 to 70 %), which greatly reduces the magnitude of the toughness of welds at subzero temperatures.

Application of nanoparticles welding nitrides TiN, VN leads to a significant increase in the proportion and intergranular polygonal ferrite (50 %), which adversely affects the toughness value (30 – 40 J / cm^2) at a temperature of – 20 °C test.

Use of nanoparticles of titanium TiO_2 and zirconium ZrO_2 oxides provides high values of tensile strength (708 and 621MPa, respectively) and toughness KCV_{-20} (60 and 72.9 J / cm^2, respectively) due to complex formation of bainite (modification TiO_2) or needle (modification ZrO_2) structures.

Furthermore a beneficial effect of inclusions of oxide (TiO_2, ZrO_2, Al_2O_3) on the structure and properties of the weld metal due to their increased resistance to dissolution in the molten metal weld pool. It has been shown that nanoparticles affect the temperature and the kinetics of phase transformation. Injection of the oxide particles leads to an increase in the temperature of the beginning of the decomposition of austenite at high temperatures bainite transformation and reduce the interval transformations.

Calculations show that the particles of regular geometric shape, ceteris paribus dissolve 20 – 30 % faster than a round. With a relatively high-speed movement of the molten metal weld pool, dissolving particles become elongated form, which affects the properties of the weld metal of high-strength low-alloy steels.

A NEW ROUTE TO SYNTHESIZE CONTROLLED-SIZE MMn_2O_4-TYPE TRANSITION METAL (M = Cd, Zn, Cu) NANOMANGANITES

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Spinel-type transition metal manganites are widely used in various field of chemistry, for example $CdMn_2O_4$ applied as sensors in NO_x or CH_3SH detection, $ZnMn_2O_4$ is known as catalysts in hydrocarbon processing, and $CuMn_2O_4$ used as oxidizing agents in oxidation of methane or exhaust gases [1 – 3]. The known classical routes to obtain MMn_2O_4-type spinels are based on high temperature (> 500 °C) solid phase reactions of various precursors, and they produce crystalline products in micrometer size.In order to obtain amorphous or highly defective nanosized spinel catalysts with superior activity, we developed a new low-temperature reaction route. Our spinel preparation is based on the solid phase quasi-intramolecular redox reactions of complexes consisting of cations with reducing ligands and oxidizing anions. Inorganic complexes containing the reducing ammonia ligand and the oxidizing permanganate anion, such as tetraamminemetal (II) permanganates $[M(NH_3)_4](MnO_4)$ (M = Zn, Cd, Cu) possessing hydrogen bonds between the ligand and anion, were proved to be the best candidates for this reaction route [4 – 7].

Generally, permanganates and inorganic ammine complexes decompose easily with oxygen and stepwise ammonia evolution, however, transition metal ammine complexes containing oxidizing anions (permanganate, perchlorate) decompose typically explosively upon heating [4] due to exothermic self-accelerating redox reactions.

The key parameters that occur and control the formation of manganites are the following:

1) the presence of a reactive hydrogen bond between the reducing ligand and the oxidizing anion, which ensures a possibility of a redox reaction between the anion and ligand even below the decomposition temperature of the complex cation or the permanganate anion;
2) low temperature to avoid the decomposition of the complex cation and the oxidizing anion; and
3) the presence of an effective heat absorbing media to remove the evolved exothermic reaction heat in order to prevent the sample from local overheating and thus the heat-induced self-accelerating decomposition.

The first condition can be determined from crystal structure data and the second and third can be ensured by using an inert liquid heat absorbing media, such as chlorinated hydrocarbons, and using lower decomposition temperature than 120 °C.

In order to avoid heat-induced self-accelerated decomposition and explosion of precursors (the decomposition reactions are strongly exothermic), the temperature of the reaction mixture has to be kept at a constant value during the all process. If the decomposition temperature is selected to be the same as the boiling point of the solvent, the evaporation heat of the solvent can absorb the exothermic reaction heat and the temperature of the mixture cannot be increased until complete solvent evaporation. Using excess solvent and adjusting the boiling point of the solvent by using vacuum, the selected decomposition temperature can easily be adjusted.

The tetraamminemetal (II) permanganates are hardly characterized compounds and the known preparative methods are either very complicated or provide very low yields [4]. In order to use these compounds as precursors, first a new effective and convenient synthesis method had to be developed. It was found that the reaction of tetraamminemetal(II) sulphates and concentrated sodium permanganate (40 %) solution produced the expected compounds in 85 – 90 % yields if a temperature gradient of + 10 / + 2 °C was used.

The precursor complexes were characterized as easily exploding compounds; upon heating, ammonia oxidation products (nitrogen oxides and water) and lower valence manganese oxides formed [4]. Since the thermal behavior of these complexes are similar, and their thermal behaviour and decomposition characteristics are key parameters in the preparation of transition metal spinel nanoparticles, the general decomposition characteristics of these materials are shown for the copper (II) complex as an example (**Figure 1**).

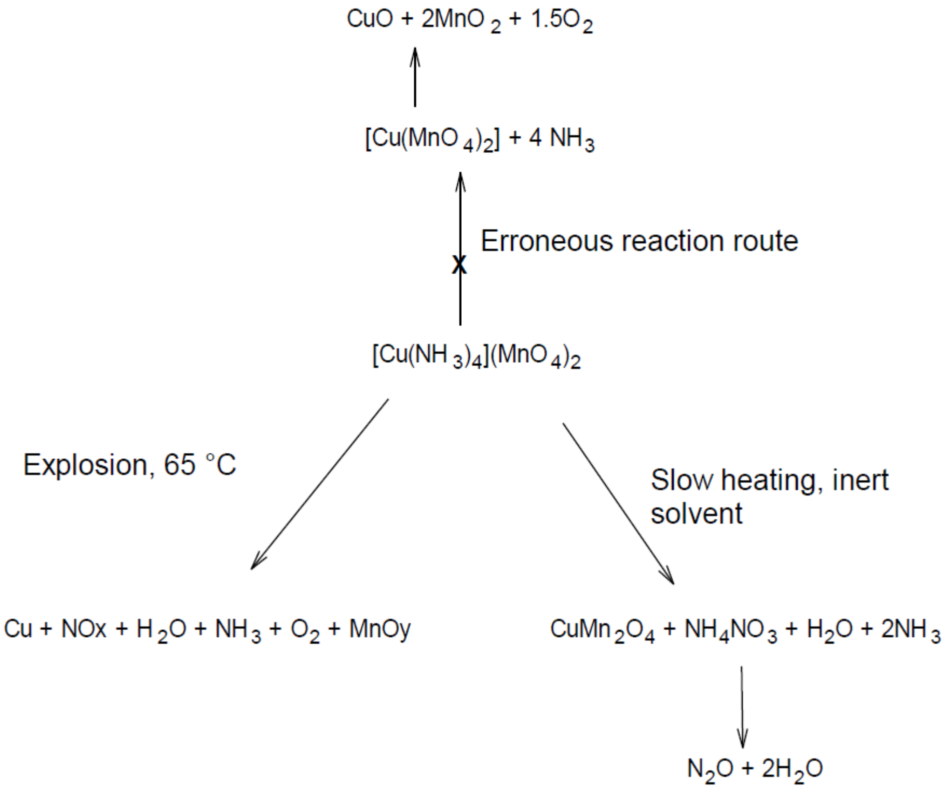

Figure 1. General decomposition characteristics of precursors shown for copper (II) complex.

We found the former data [8] declared about thermal decomposition of tetraammine copper (II) permanganate by stepwise loosing ammonia and oxygen evolution was erroneous. Therefore, we found a new method to prepare $CuMn_2O_4$ spinel from the precursor tetraammine copper (II) permanganate.

Tetraammine copper (II) permanganate is described as a purple crystalline compound, which decomposes with explosion at ~ 65 °C. Diluting it with inert material (alumina) and applying a very low heating rate (0.2 °C / min), the decomposition takes place at ~ 80 °C and results in two moles of ammonia and one mole of water loss, but without oxygen evolution [5]. This reaction route leads to the formation of amorphous $CuMn_2O_4$ and NH_4NO_3. However, the products cannot be separated from the alumina diluent, therefore we used carbon tetrachloride as heat-absorbing media.

Characterization of nanosized manganites

The transition metal manganites (M = Zn, Cd, Cu) formed in the quasi-intramolecular redox reaction of tetraammine metal (II) permanganates formed in an almost stoichiometric reaction with high yield (above 95 %) during prolonged heating (2 h) were proved to be amorphous material. The TEM picture of the product formed in this reaction in an intermediate stage shows the residual crystalline precursor embedded into the amorphous matrix (**Figure 2**).

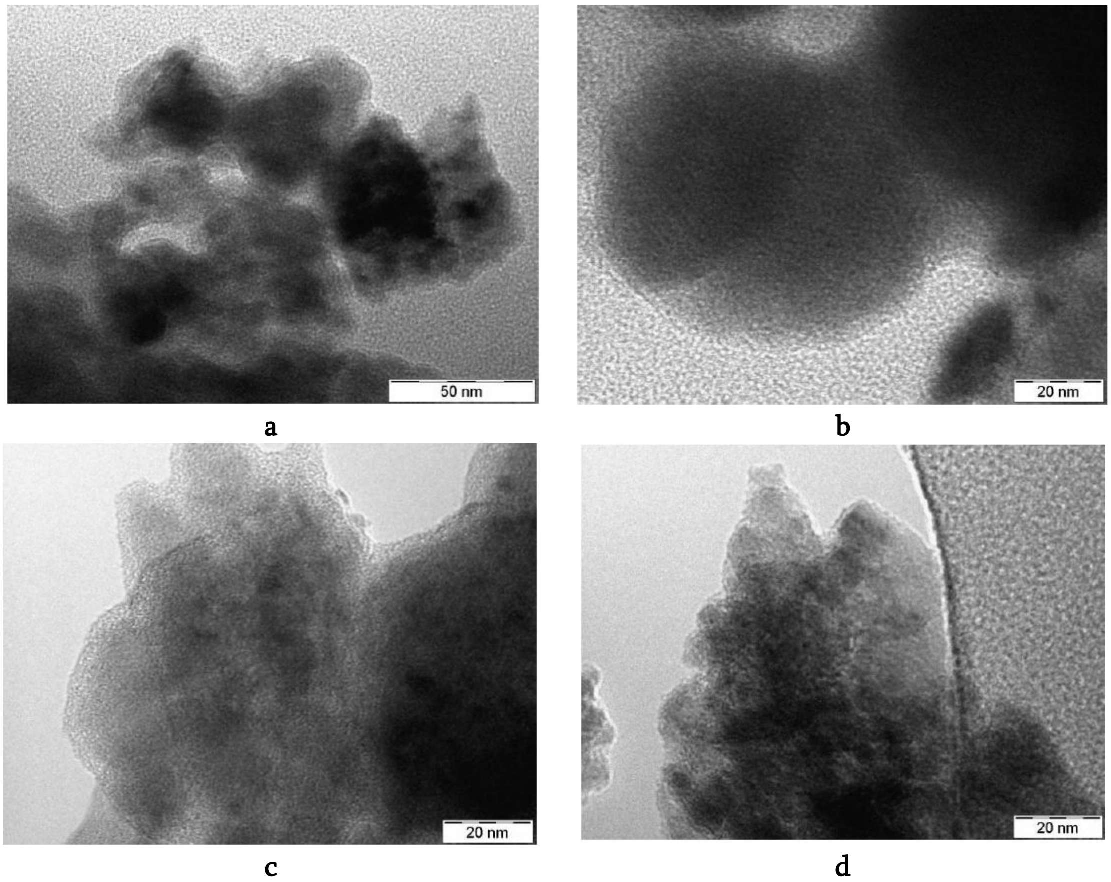

Figure 2. a – d TEM pictures of the amorphous reaction product ($CuMn_2O_4$) with embedded precursor crystals.

The formation of the amorphous phase is the consequence of the mechanism of the reactions. During decomposition the heavy atoms (transition metals and Mn) of the precursor tetraammine copper (II) permanganate loose their ammonia ligands. As a result the coordination sphere of metals is destroyed and the material is no longer crystalline. Heating induces the rearrangement of oxygen around metals and crystalline spinel forms. Its size can be controlled with the heating temperature (**Figure 3**). For example, the size of the crystallites at 230 °C was found to be 2 nm, whereas heating at 500 °C resulted in 100 nm size crystallites.

The described reaction route is general, similar result was found in case of bis(pyridine)silver (I) permanganate, where the redox reaction center had also a hydrogen bond between the a-CH of one of the pyridines and permanganate oxygen, while the other pyridine ligand liberated without oxidation in the decomposition reaction of $[Agpy_2]MnO_4$ [9].

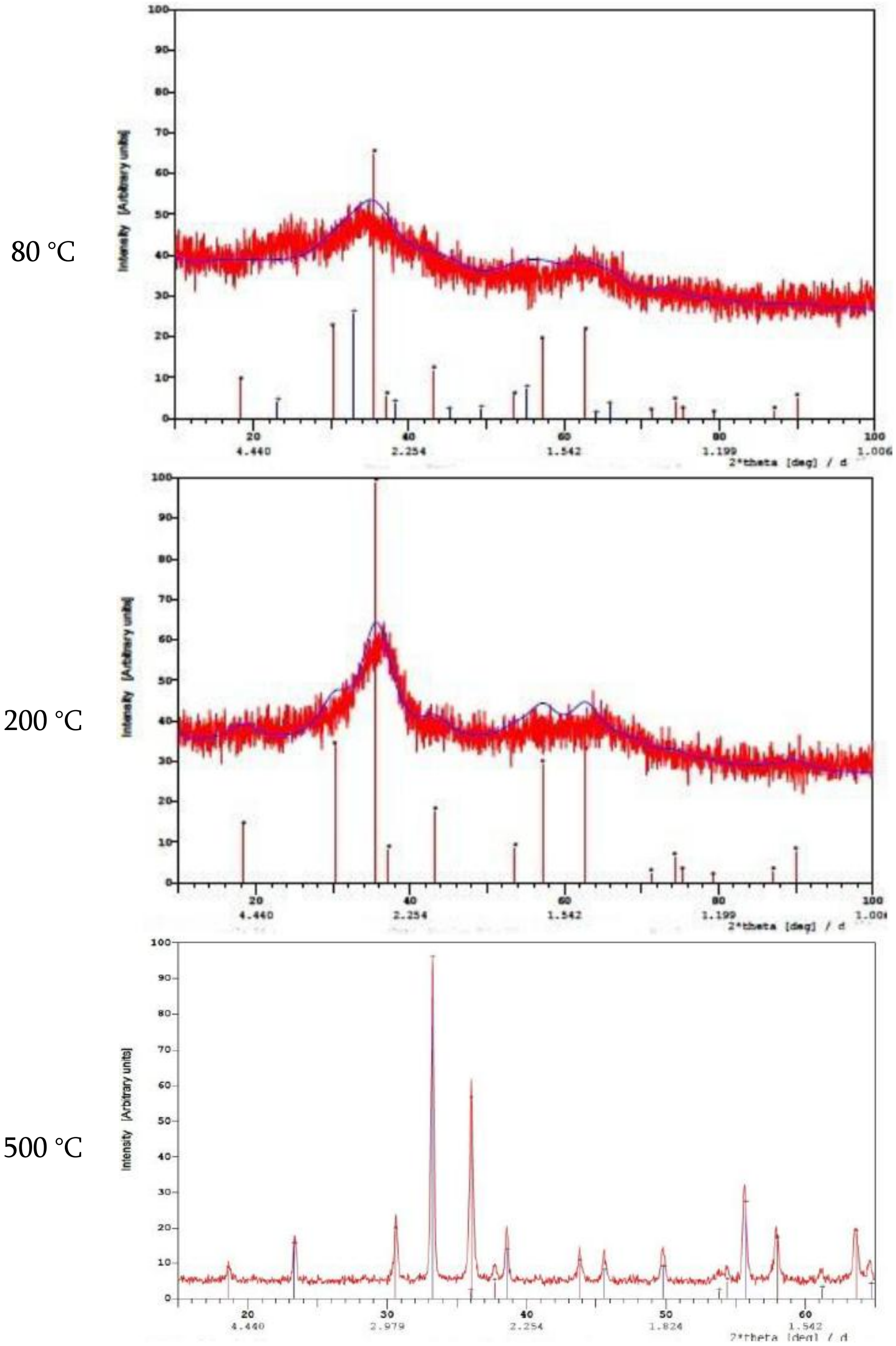

Figure 3. XRD of nanosize (89 and 200 °C) and crystalline (500 °C) $CuMn_2O_4$.

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BRAIN TUMOR RESEARCH METHODS

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The human brain is the center of the nervous system. In the brain, as well as the spinal cord is placed in a white and gray matter. White conductive substance ways to generate. Separate clusters of gray substance – nuclei – in the form of a white substance inside deployed. 14 billion neurons in the cortex.

Discovered tumors on contrast enhanced mprage images. Using the mprage information, located tumor on the 6 maps (MK, MD, TT, SD, KP, and FA). Searched the highest intensity region of the mass on TT map and then measured the intensity values in the same voxel on the rest of the maps. Created the table of the intensity values for all 6 maps of 44 patients. Calculated the correlation with these maps.

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TO THE KINETICS OF QUANTIM DYNAMIC SYSTEMS INTERACTING WITH A THERMOSTAT (BOSON FIELD)

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New exact generalized closed quantum evolutionary (kinetic) equations for the equilibrium double-time correlation functions and statistical operator (density matrix) of a quantum dynamic system interacting with a thermostat (heat bath) were derived in the case of linear as to the Bose-amplitudes it's interacting with the phonon (boson) field. The random phase approximation (RPA, factorizing initial condition) has not been used to derive these equations. The projection operator technique is used for excluding the dynamical variables of a thermostat (boson amplitudes) from the derived kinetic equations. The generalized equations of evolution with excluded thermostat operators follow from exact obtained equations in case of weak (sub)system–thermostat interaction. The collision integrals of these equations include explicitly both the dissipative terms describing the system's dynamics and the terms responsible for the time evolution of the initial correlations.

As an application of this approach the uniform theory of Froehlich polaron mobility and conductivity in the wide frequency range of weak external fields developed. It reproduces the generalized Osaka result at small frequencies and generalized Feynman-Hellwarth–Iddings–Platzman (FHIP) result at high frequencies. Such uniform theory was not developed until now.

The derived evolutionary equations are used also to analyze the kinetic and linear transport phenomena in exactly solvable model of the quantum dissipative system: A quantum Brownian particle, dynamics of which is described by the Caldeira–Legget Hamiltonian.

The generalized Bogolubov's lemma for a dynamical system interacting with the boson (phonon) field is proved and used for excluding the dynamical variables of a thermostat (boson amplitudes) from the derived kinetic equations. The relaxation time of the correlation functions, the mobility of the Brownian particle were calculated and the in fluency of the initial correlations is discussed.

CHARGE TRANSPORT PECULIARITIES IN NANOCRYSTALLINE HETEROPOLYTYPE SiC FILMS OBTAINED BY DIRECT ION DEPOSITION

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Electronic devices based on semiconductor heterostructures are used extensively in different areas of science and technology [1]. One of the semiconductor materials most promising for operation under the conditions of external attacks is silicon carbide. The heterostructures SiC created by the layers of nanocrystalline SiC of different polytypes were grown by the method of direct ion deposition [2]. The aim of the present work was to study the mechanisms of charge transfer in the nanocrystalline heteropolytype SiC films, deposited on leucosapphire single-crystalline substrates. The average size of the nanocrystals in the heterostructures SiC was 5 – 10 nm. To clarify the mechanisms of charge transport in the obtained films there was studied the temperature dependence of their electrical conductivity σ. The electrical measurements were performed by the four-contact method at direct current.

The electrical conductivity of the heteropolytype film is the sum of the conductivity values of the parallel channels $\sigma = \sigma_1 + \sigma_2 + \sigma_{hj}$, where σ_1 and σ_2 are the conductivity of the monopolytype regions which form the heteropolytype film, σ_{hj}, the heterojunction conductivity. It was found that main contribution to the electrical conductivity of the films belongs to the contact region of the heterojunction, i.e. condition $\sigma_1 + \sigma_2 << \sigma_{hj}$ is fulfilled. This is due to the fact that in the contact region the charge transfer is realized by the multistep tunneling via discrete energy levels with close energies. These discrete energy states arise in the forbidden band due to the dimensional quantization. It was established that the characteristic energy of the charge transfer process is of the order 10 meV.

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PARAMAGNETIC PROPERTIES OF THE PYROLYZED NANOSTRUCTURED CARBON MATERIAL (COAL)

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Coal is a nanostructured natural material, where the physical-chemical properties depend from the stage of metamorphism. Metamorphism is a natural transformation of structure the coal under pressure and temperature.The stage of metamorphism is estimated by a variety amount volatile substance (V^{daf}).The coal structure is considered to consist of the nanoclusters with the ordered distribution of carbon atoms (aromatic area) and the amorphous bridges between carbon nanoclusters containing hydrocarbon CH_n chains (aliphatic area) [1, 2]. The process of pyrolysis demonstrates the partial destruction of organic bonds in the aromatic and aliphatic areas with changing physical-chemical properties, including paramagnetic.

In this paper, it was researched influence paramagnetic oxygen O_2 on the paramagnetic properties a gaseous type of coal with different amount of volatile substance ($V^{daf} = 39 – 46$ wt. %.) after vacuum annealing at $T = 650 – 700$ °C.

EPR spectra of coal after vacuum annealing consist of a two resonance lines L1, L2, which have Lorentz shape.The broad line L1 and narrow line L2, which corresponds to the non-compensated electron spins within two areas in the coal structure: the carbon nanoclusters (aromatic area) and long one-dimensional hydrocarbon molecules of CH_n type (aliphatic area) [3].The weakly increasing width of EPR line after vacuum annealing related to dipole–dipole interaction with paramagnetic oxygen O_2 [4].

At first, time was registered untypical behavior paramagnetic centres of coal with an interaction of oxygen molecule O_2 after vacuum annealing. The anomalous increase of the width ($\Delta H_{pp} \sim 250$ G) of L1 line related to interaction unpaired electrons of coal with paramagnetic O_2 after vacuum annealing. This behavior of width L1 line was explained by a large amount open pores of coal, which were created by vacuum annealing. During of time the intensity and width of an L1 line of coal with contacting of oxygen after vacuum annealing slowly decreased. The intensity of L2 was increased but the width did not change.The decrease of paramagnetic concentration of centres in the aromatic area of coal after vacuum annealing related to creating weakly chemical bonds with oxygen.The increase of paramagnetic concentrations of centres in the multi-ring aromatic hydrocarbon and aliphatic area by structure relaxation of bound with chemical reactions and diffusion free radicals.

Finally, we investigated the same behavior of paramagnetic centres of coal with interaction of vapor of water. The interaction paramagnetic centres of coal with a vapor of water proceeds faster that with oxygen.

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MICROWAVE EMITTING SPIN-ORBIT-DRIVEN MAGNETIC DYNAMICS IN MULTILAYER NANOSTRUCTURES

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The intercoupling between a spin current and magnetic state in magnetic nanostructures underlies of the current-induced manipulation by magnetic dynamics and vice-versa, the magnetic state-induced manipulation by the spin current [1, 2]. The spin current can be converted from an input current under the internal effective magnetic fields of interactions of a different origin (including $s-d$ exchange and spin-orbit interactions) with corresponding features of the action of the spin torque on the magnetic states and their dynamics. These spin torque can cause switching and precession of the magnetic order vectors. The frequency of the magnetic dynamics is determined by the magnitude of magnetic exchange interaction, which is the largest for antiferromagnetic materials. Therefore, the prospect of obtaining the technological magnetic nanostructures with low threshold incoming currents, low power consumption and controlled high frequencies is related to the spin-orbit generation of the spin current and magnetic nanostructures with antiferromagnetic (AF) exchange interactions.

Generally, the spin-orbit interaction, resulting in the spin current, includes the volume spin Hall (SH) effect of the transverse (relatively to an incoming current) deflection of electrons with opposites spins in opposite sides and the interface Rashba spin-orbit (RSO) effect of the spin splitting of an electron disperse along an electron wave vector. The impact of the spin current on the magnetic states realizes via the spin torque $\mathbf{T}$ consisting of so-called a field-like and dumping-like part $\mathrm{T}_{\|}$ and $\mathrm{T}_{\perp}$, respectively, which are related to the effects of magnetic order vector switching and precession dumping or antidumping. The field-like torque $\mathrm{T}_{\|}$ originates predominantly from the spin-orbit coupling at the interface, in conjunction with the perturbation of the electron distribution function. The torque $\mathrm{T}_{\perp}$ originates predominantly from the perturbation of electronic states by the applied electric field.

The current spin-orbit-controlled microwave oscillation realizes in magnetic nanostructures composed of a heavy metal nanolayer (Pt, Ta) with the strong enough spin-orbit interaction and the adjacent active magnetic with antiferromagnetic exchange interaction (based on ferri- or antiferromagnetic interactions). The Landau-Lifshitz-Gilbert-Slonczewski dynamic model for the magnetic sublattices with AF exchange interaction together with the feed-back from the combined effect of the SH and inverse SH effect of the spin pumping with spin backflow, results in conditions of steady-state microwave spin torque oscillations. The latter combined with a conversion into the ac voltage via anisotropy magnetoresistance effect can lead to nano-sources of THz radiation.

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HYPERTHERMIC TREATMENT OF TISSUES BY USING OF Fe_3O_4 AND $NiFe_2O_4$ NANOPARTICLES

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The magnetic nanoparticles for hyperthermic treatment of cancers have gained significant attention in recent years. For efficient use of the hypothermic method it is necessary to locate the magnetic nanoparticles in a predetermined region and thereafter reheat them using alternating high-frequency electromagnetic field to strictly predetermined temperature. The speed and the maximum heating temperature of the magnetic nanoparticles depends not only on the amplitude and frequency of the used alternating electromagnetic field and heat conditions, but also on the electromagnetic and geometric characteristics of these nanoparticles. Typically, at the certification of magnetic nanoparticles, their size and magnetic susceptibility are indicated. However, due to the fact that during hypothermia for localization of magnetic nanoparticles in the area of a diseased organ a strong permanent magnetic field is used, the characteristics of these nanoparticles can strongly vary. The sizes of nanoparticles can be increased due to clumping and conglomeration in the magnetic field. A permanent magnetic field can also lead to a change of a high-frequency magnetic susceptibility due to the anisotropy of magnetic nanoparticles and to the difference in the coefficients of the longitudinal and transverse attenuation of the magnetic moment.

In the present work we study the influence of a permanent magnetic field on the high-frequency magnetic characteristics of Fe_3O_4 and $NiFe_2O_4$ at different conditions (dry powder and in liquids with different viscosities). The geometric dimensions are the following: for Fe_3O_4 nanoparticles these are 10 – 40 nm with a maximum density of the distribution function near 16 – 20 nm; for nanoparticles $NiFe_2O_4$ – 30 – 150 nm with a maximum density of the distribution function near 40 – 60 nm. The field was applied both along the coil axis and perpendicularly to the coil axis, i.e., perpendicularly to the high-frequency measuring field.

The results of the investigations demonstrated that the permanent magnetic field affects the high-frequency magnetic susceptibility of an ensemble of nanoparticles in powder, water, and glycerin. A permanent magnetic field also changes the speed and efficiency of heating of a nanoparticles ensemble. Moreover, this effect depends on the relative orientation of a permanent and high-frequency magnetic field. In addition we have established that the size of a magnetic susceptibility of the investigated nanoparticles χ changes in a static magnetic field. The value of χ increases for nanoparticles $NiFe_2O_4$, when the direction of a static magnetic field coincides with the direction of measured variable field. In opposite case, when the direction of the static magnetic field is perpendicular to the direction of the measured variable field the value of χ reduces. For Fe_3O_4 the value of χ decreases for both, the in parallel and perpendicular directions of the static magnetic field to the measured variable field. The received dependence can be explained by the anisotropy of magnetic nanoparticles (shape anisotropy or of the crystal structure anisotropy).

MECHANICAL ALLOYING AND PROCESSING OF NANOMATERIALS BY HIGH ENERGY MECHANICAL MILLING

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Nanocrystalline materials or nanopowders are the bridge between bulk materials and atomic structure and characterized by a large volume fraction of grain boundaries, which can allow the significantly improvement of the properties of powders such as the mechanical, chemical and physical properties compared with conventional coarse-grained polycrystalline materials. As the grain size is decreased, an increasing fraction of atoms can be ascribed to increased grain boundaries. Therefore, nanocrystalline materials may exhibit increased strength / hardness, improved toughness, reduced elastic modulus and ductility, enhanced diffusivity, higher specific heat, enhanced thermal expansion coefficient, and superior soft magnetic properties in comparison with conventional polycrystalline materials. This has lead been the performing of widespread research in this area, and developing of suitable advanced tools for processing and characterization of them. Among the nanopowder synthesizing powder metallurgy methods, in recent years, mechanical alloying (MA) has recognized as an attractive solid state nano powder fabrication method, which explores the simple operations for mass production and low economical processing method. The actual process of MA starts with mixing of the powders in the right proportion and loading the powder mix into the mill along with the grinding medium. This mix is then milled for the desired length of time until a steady state is reached when the composition of every powder particle is the same as the proportion of the elements in the starting powder mix. The milled powder is then consolidated into a bulk shape and heat treated to obtain the desired microstructure and properties. Thus the important components of the MA process are the raw materials, the mill, and the process variables. In this paper fundamental aspect of MA and effected factors involved in the selection of raw materials, types of mills, and process variables is overviewed. Except than the well known examples, the paper has also extended with the concerning with the performed researches on the production of MgB_2 by use of high-energy mechanical milling methods. In the synthesis of MgB_2, as bulk, wire or thin film forms the structure of the precursor powders is very critical to obtain good superconducting properties. Ductile deformation behavior at low temperatures and small grain size which enhance the grain boundaries, are accepted as a favorable precondition to achieving a high quality MgB_2.

THE MODELING OF KINETIC PROCESSES IN THE NANO-LAYER SENSOR OF THERMOELECTRIC SINGLE PHOTON DETECTOR FOR X-RAY PHOTONS

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The increased interest in recent years to sources and detectors of single photons is due to remarkable progress in different areas of science and technology. The thermoelectric single-photon detector (TSPD) is one of the real competitors to superconducting detectors for single photon detection [1, 2]. The TSPD can also serve as a basis for the development of a new generation of measuring systems for applications in quantum electronics, astrophysics, high energy physics, quantum informatics, telecommunication systems, quantum metrology, medicine, homeland security, elemental microanalysis, analysis of defects in microchips, etc.

The TSPD operation principle is based on photon absorption by absorber as a result of which a temperature gradient is generated on the edges of the sensor [3]. Photon detection becomes possible by measuring the potentials' difference, emerging between the two absorbers.

The results of computer simulation of processes of heat distribution in the multi-layer sensor of thermoelectric detector after UV single photon absorption are presented. The multi-layer sensor consists of a photon absorber (tungsten), which is deposited on the thermoelectric layer (thermoelectric with high figure of merit at helium temperatures) and the latter is deposited on the electrically conductive layer of heat sink. This "sandwich" is located on a dielectric substrate, on which are also set electrical contacts to count the potential difference ΔU, generated between the absorber and the heat sink by the absorbed photon. The calculations were carried out by the matrix method for differential equations [4], using parameters for the tungsten absorber and thermoelectric nano-layer made of (La,Ce)B_6 or CeB_6 hexaborides. Changing the thickness of absorber and thermoelectric layer we can modified the parameters of sensor such as count rate and energetic resolution.

According to the results of computer modeling presented in this paper it can be stated that detection of single photons of 1 keV energy and the possibility to define their energy with accuracy no less than 1 % is realistic. The count rate exceeding 200 GHz can be achieved.

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NANO-LAYER SENSOR FOR SINGLE-PHOTON DETECTION IN A WIDE RANGE OF THE ELECTROMAGNETIC SPECTRUM

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The results of computer simulation of heat distribution processes taking place after absorption of single photons of 1 eV – 1 keV energy in nano-layer sensor of the thermoelectric detector are being analyzed. Different geometries of the sensor with tungsten absorber, thermoelectric layer of cerium hexaboride, lanthanum-cerium hexaboride and tungsten heat sink are considered. It is shown that by changing the sizes of the sensor layers it is possible to obtain transducers for registration of photons within the given spectral range with required energy resolution and count rate. It is concluded that, as compared to the single layer sensor (**Figure 1a**), the three-layer sensor (**Figure 1b**) has a number of advantages and demonstrate characteristics that make possible to consider the thermoelectric detector as a real alternative to superconducting single photon detectors.

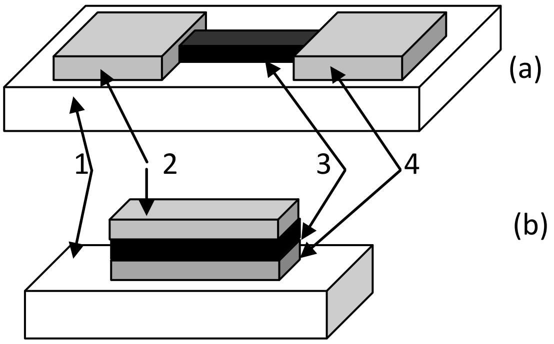

Figure 1. Single layer (a) and three-layer (b) sensors design:
1 – substrate, 2 –absorber, 3 – thermoelectric nano-layer, 4 – heat sink.

The obtained results allow the following conclusions to be done:

1. Following computer simulation, the three-layer TSPD sensor may register individual photons in a wide range of the electromagnetic spectrum from 1 eV to 1 keV, providing energy resolution of not less than 1 % and count rate from tens gigahertz to terahertz.
2. For solution of a wide range of different tasks the ratio (energy resolution) / (count rate) can be varied by changing the geometric sizes of the sensor.
3. TSPD with a three layer sensor can present a real concurrence to superconducting detectors.

The authors hope that the present publication will attract attention to thermoelectric detectors and that the experimental results on TSPD research will appear soon, since following the results of computer simulation this is quite a perspective direction.

INVESTIGATION OF NANOSKIN PECULIARITIES FORMED DURING OXIDATION OF LIQUID GALLIUM SURFACE

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Membrane technology of obtaining super-pure ($7N^+$) gallium and conservation of big masses (not droplets) of its melt in overcooled liquid state at room and lower (≤ 20 °C) temperatures for practically unlimited period of time is already known [1 – 3]. Therefore, such melt represents unique model object for investigation of oxidation process of metal with atomically flat surfaces.

In the given work, formation kinetics and structure of nanoskin obtained on the super-pure ($6N – 7N^+$) gallium melt surface during oxidation in air at temperature range 20 – 50 °C is studied by methods of Precision Weighing, SEM-EDX and Auger-electron Spectrometry. It is shown that, as a result of penetration of oxygen atoms released by dissociative adsorption, the concentratedly layered subsurface with 5 – 6 atomic diameter thickness transforms to elastic nanoporous Ga_2O solid skin, such as continuous precise coatings of equal thickness (~ 15 Å), on the whole surface of the melt. The further growth of the mentioned skin thickness, generated in the first seconds, obeys more retarded kinetics and after few hours its thickness reaches ~ 50 nm. Depending on the nanoporous condition of the generated skin and that it is lyophilic towards melt, gallium melt of some mass (20 – 50 g) encapsulated in the given skin naturally generates system of membrane module “melt–membrane–atmosphere”, in which extraction of impurity atoms from melt into the reactive membrane is ongoing. Experimentally is shown that growth of the membrane thickness occurs too slowly during photostimulated oxidation process in the atmospheric conditions and after a dozen hours, upon reaching ~ 1000 nm thickness, it practically stops.

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III–V SEMICONDUCTOR NANOSTRUCTURE FOR SOLAR CELLS

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Solar Cells (SC) are devices that convert sunlight directly to electricity. The most important characteristic of solar cell is conversion efficiency. Compound III–V semiconductor solar cells have experimentally achieved efficiencies of more than 40 % [1, 2], it is highest efficiencyavailable for Photovoltaic (PV) SC today and its further increase is a key for massive utilization of solar energy worldwide.

There are two main design techniques for inorganic III–V semiconductor PV solar cells: multi-junction solar cells (MJSCs) [3] and intermediate band solar cells (IBSCs) [4]. In MJSCs a number of semiconductor material junctions are connected in-series, each of them designed for efficient absorption of a section of the solar spectrum appropriate to its band gap. In IBSCs an intermediate energy band (IB) is introduced into the band gap of the single junction semiconductor material for increase number of possible electron transitions.

Replacement of bulk semiconductor with the nanostructured materials in the active region of PV SC is very promising for dramatic improvement of such characteristics as efficiency, size and cost of cells [5 – 7]. Many theoretical studies were carried out for design of new generation solar cells with quantum dots (QD); various methods of fabrication III–V semiconductor QDs were developed [8 – 9]; but there still is a huge space for future development and any experimental achievement in this direction is important.

In this work, we describe a new, simple method of preparation of nanocrystals on the III–V semiconductor surface. This method includes electrochemical deposition of III group metals (In, Ga, Al) on electrochemically etched semiconductor surface. The chlorides of metals are used for In and Ga deposition as described in [10]. After metallization GaP wafer are annealed in hydrogen during 3 – 10 min at the various temperatures for formation of InP nanocrystals on GaP surface. Influence of annealing temperature on the electro-physical characteristics of In / GaP system is investigated and possible mechanism of interactions between metal and semiconductor during forming of InP nanocrystals are discussed. Application of obtained structures for MJSCs predicted.

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ACTIVITY OF *VITEX* LEAVES EXTRACTS IN SYNTHESIS OF SILVER NANOPARTICLES

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Recently, green synthesis of metal nanoparticles (NPs) using plant extracts has attracted a great attention [1]. Metal nanoparticles are known to be the promising materials for electronics, material science, catalysis, biology, medicine. Use of plants extract for NPs production provides the synthesis with beneficial requirements: mild temperature and pH, non-toxic and cheap reducing / stabilizing agents [1 – 4]. Many kinds of plants were found to be a valuable source of various active compounds (phenols, flavonoids, sugars, etc.) which are reducing / stabilizing agents for NPs synthesis [2 – 5]. Plants of *Vitex* genus seem to be perspective raw material for green synthesis of NPs, too, due to high content of compounds with antioxidant / reducing properties [6].

Silver nanoparticles (AgNPs) colloids were synthesized using leaves extracts from three different species of *Vitex* genus, namely: *Vitex cannabifolia*, *Vitex agnus-castus*, *Vitex negundo*. The biologically active substances were extracted from the leaves with a 70% ethanol solution. Composition of the extracts was studied using LDI mass spectrometry, HPL chromatography, and methods of chemical analysis. To characterize antioxidant/ reducing properties of the extracts, the Folin–Chocolteu method and DPPH test were applied. Synthesis of AgNPs was carried out using 1 mM $AgNO_3$ aqueous solution at temperature of 40 °C under continuous stirring. The formation of AgNPs in the reaction mixture was monitored by the changes in intensity of 430 nm absorption band in the UV spectra, corresponding to AgNPs plasmon resonance.

All the *Vitex* extracts were found to contain high amounts of antioxidant/reducing agents. All the extracts revealed significant activity in AgNPs synthesis, with the ability of the extracts to reduce Ag^+ ions being correlated with the extracts composition and their antioxidant/ reducing properties. Extract from the *Vitex cannabifolia* leaves with the smallest phenol content had the lowest activity in AgNPs synthesis. Extract from the *Vitex negundo* plants with the highest phenol content showed the fastest reduction of Ag^+ ions during first several days of the reaction while the extract from *Vitex agnus-castus* leaves with the highest flavonoids concentration revealed comparable activity in AgNPs synthesis in spite of much smaller phenol content.

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THE EFFECT OF ADDITIVES OF THE FOURTH GROUP OXIDES ON THE SINTERING KINETICS OF TETRAGONAL ZIRCONIA NANOPOWDER

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Ceramics based on tetragonal zirconia nanopowders 3Y–TZP worldwide known for its excellent physical and mechanical properties such us high strength, toughness and hardness and widely used in medicine, optical fiber connectors, grinding media, and precision parts. It is really important to clarify how we can control the properties of ceramic microstructures by doping modifying additives [1, 2]. Today it is urgent to study the influence of the concentration and nature of the additives and their effect on sintering and products properties.

In the present paper the authors investigated the effect of small amount additives SiO_2, SnO_2 and TiO_2 on the initial sintering stage of tetragonal zirconia nanopowders. It has been found that different additives differently influence on phase composition, crystallite size and agglomeration degree of zirconia nanopowders which were manufactured by co-precipitation method.

The sintering behavior of 3Y–TZP with and without a small amount of SiO_2, SnO_2 and TiO_2 additions was investigated using the dilatometric data and analytical method for determining the sintering mechanism [3]. The shrinkage behavior of all nanopowders was measured under constant rate of heating (CRH).

Table 1. The order of diffusion mechanism and activation energies of sintering.

Nanopowders	n	Q (kJ / mol)	Sintering mechanism
3Y–TZP (DIPE)	1/2	667	VD
3Y–TZP–2 wt. % SiO_2	1/3	757	GBD
3Y–TZP–2 wt. % SnO_2	1/3	979	GBD
3Y–TZP–2 wt. % TiO_2	1/3	1120	GBD

The sintering mechanism changed from volume (VD) to grain boundary diffusion (GBD) by addition 2 wt. % SiO_2, SnO_2 and TiO_2 as shown in **Table 1**.

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INVESTIGATION OF OPTICAL PROPERTIES OF HYBRID NANOPARTICLES SYNTHESIZED BY LASER ABLATION IN LIQUIDS

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In the present work the optical properties of colloidal hybrid nanoparticles in metal–semiconductor and metal–metal systems fabricated by pulsed laser ablation in pure water, is considered. The red-shifted photoluminescence of (Si–Ni) system which is located in the blue spectral range with the center of wavelength at 460 nm has been registered. This phenomenon has been explained by considering the electrostatic Stark effect in the Coulomb field of the charged Ni nanoparticles [1]. The Au, Ti, Ni and Cu, as well as Au–Ag and Au–Cu hybrid metal nanoparticles also were formed in the liquid medium. The change of wavelength of plasmon resonance of hybrid metal nanoparticles under such circumstances has been registered. The laser surgical procedures of welding and ablation after the colorations of biotissue samples with metal nanoparticles have been studied. The effectiveness of laser ablation after addition of nanoparticles was approximately on 4 – 5 times larger than for the native sample.

The significant applications of considered systems mainly concern the nanobiology and nanomedicine.

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InP BAZED NANOMATERIALS FOR TELECOMMUNICATION

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III–V semiconductor materials GaAs, InAs, GaP, InP, etc. have a good optical and electrical properties for high performances photonic and electronic devices. Modification of the density of states due to the materials dimensionality of semiconductor nanostructures (quantum well (qW), quantum vire (QW) and quantum dots (QDs)) is responsible for many of the improvements in the properties of devices, including higher gain of lasers, lower threshold current densities and a smaller temperature sensitivity. InP is a direct bandgap (1.344 eV) semiconductor with exciton Bohr radius of 10 nm. InP gives strong light emission at a near infrared wavelength. The emission wavelength of InP nanocrystals (NCs) can be tuned throughout the whole visible and near-infrared range by changing their size. Therefore, InP NCs are very promising for use lighting and display applications. QD infrared photo detectors are an important technology in the field of infrared detection for military applications. Stranski–Krastanov (SK) growth mode is the most often utilized self-organized nanostructure growth technique [1]. Chemically synthesized InP NCs are less toxic alternative to CdSe-based nanocrystals [2]. The formation of InP nano crystals by droplet epitaxy using molecular beam epitaxy is described in [3]. Single-photon emission from InAs / AlGaInAs / InP quantum dots (QDs) at wavelengths above 1.5 μm that are compatible with standard long-distance fiber communication, is demonstrated [4].

The dependency of the electric and photoelectric characteristic on the annealing temperature (150 – 350 °C) of In / GaP Schottky Barrier was investigated in [5], and new region of the strong photosensitivity in near infrared region, was related with formation of a new nanostructured material on the surface of GaP via interaction between metal (In) and semiconductor (GaP) during annealing of the In / GaP. In this work the mechanism of formation of InP NCs on the surface GaP is discussed analysing of our experimental results and of results of research works from literature. InP based nano structural devices for optical telecommunication application is studied and, a new simple technology of fabrication of InP NCs is described here.

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THERMOSTABLE PHOSPHATE MATRIX FOR NANOCOMPOSITE MATERIALS

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A wide range of thermostable materials based on phosphate binding compositions (i.e. phosphate matrix) and operating at temperatures up to 1800 °C have been successfully prepared [1, 2]. In recent years due to rapid improvement of the materials production process which assume the utilization of nanosized functional fillers the using of phosphate matrix for the development and preparing of thermostable nanocomposites are of great interest [3].

In present communication we report about the results on the fabrication and research of different thermostable composites based on phosphate matrix and containing such functional nanosized fillers as aluminum oxide Al_2O_3, aluminum nitride AlN, silicon carbide SiC, some boron compounds (B amorphous and polycrystalline, BN, B_4C), and CNT.

Phosphate composites consist of a binding substance and fillers, which are mixed in a definite proportion just before application to a surface or making a required pattern. Binders may be phosphoric acid or alumophosphate solutions modified with various additives. As to fillers, one may use oxides of aluminum, chromium, iron, titanium, zirconium, or silicates of aluminium and zirconium, or minerals of natural origin. In certain cases some waste products can be used and the proportion of the latter items in the new materials could exceed 50 % by mass. After the patterns' molding and shaping, or applying the composition (as a coating or paint), hardening of phosphate composites occurs at room temperature (which may take from several hours to several days), and, if necessary, it may be achieved by thermal treatment of compositions up to temperatures 50–300 °C.

Specific application area of the phosphate nanocomposite materials, conditions of their operation, and attaining of definite physical, chemical and mechanical characteristics are determined by the composition and proportions (i.e. ratio) of main components: the binder and the fillers. Thus, depending on the filler nature, phosphate composites may perform as radio-transparent or radio-absorbing materials, electro-conductors or dielectrics, thermo-conducting or thermo-insulating materials as well as materials for ionizing radiation protection (shielding).

Phosphate composite materials are non-combustive, nontoxic and environmentally safe. Their manufacture is waste-free and does not need any complicated equipment, thus it can be organized at any enterprise of building industry. The available application fields of the thermostable materials based on phosphate binding compositions are: aviation and space industry, metallurgy, ceramics industry, production of refractories and building materials.

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Ag vs Au IN CORE–SHELL TYPE NANOCOMPOSITES $FeFe_2O_4$ & PRECIOUS METAL: PUTATIVE BACKGROUND OF DIFFERENT ACTIVITY IN BIOLOGICAL ENVIRONMENT

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Nanocomposites with magnetic core material and precious-metal shell are considered as promising medication in fighting against infections with high resistance to antimicrobials [1].

Earlier, we have shown free radical interfering, bactericidal, and immunomodulating activity of nanocomposites comprising iron oxides core and Ag^0 or Au^0 shell [2 – 5]. During these structures producing by means of so-called rotation-corrosion dispergation procedure, various size and shape nanoparticles could be received depending on the initial pH and precious-metal ions concentration in the system [6, 7].

X-ray diffraction analysis of the samples revealed the presence of magnetite – $Fe^{II}Fe^{III}O_4$ (Fe_3O_4), lepidocrotite – γ-$Fe^{III}OOH$, and metallic silver or gold. The data obtained using X-ray fluorescence spectroscopy and zeta potential measurements enabled calculation of reaction equilibrium constants as follow: $K_{Ag} = 10^{0.47}$ for silver and $K_{Au} = 10^{37}$ for gold. Consequently, the reaction system with Ag^+ has pH and concentration limits, which are likely to increase the proportion of needle-shaped nanoparticles and islet-like shell formation in spheroidal ones. In contrast, $AuCl_4^-$-containing system provides the output of predominately spheroidal nanostructures with dense shell. Foregoing consideration was also confirmed by relevant TEM-images.

Recent evidences of innate silver and gold nanoparticles electrochemistry, which determine their catalytic activity and core–shell interaction in similar nanostructures [8, 9] can explain the mechanism of biological activity attributable to $FeFe_2O_4$ & Precious Metal nanocomposites.

Hence, in biological environment, $FeFe_2O_4$&Ag^0 nanocomposites might be preferred to maintain free radical generating processes, whereas $FeFe_2O_4$ & Au^0 would rather inhibit them.

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THE INTERACTION OF COPPER AND COBALT SPINEL FERRITE NANOPOWDERS WITH ORGANIC LIQUIDS CONTAINING OLEIC ACID

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Nowadays the usage of oleic acid as a stabilizing agent for the obtaining of colloidal stable oxide and ferrite nanoparticles has been well known [1]. Usually oleic acid is added into chemical mixtures of the initial reagents at the time of a synthesis procedure [2]. However the chemical treatment of the oxide powders by various organic liquids (hexane, chloroform, dichloromethane) containing an admixture of oleic acid takes place among other methods of nanoparticle's stabilization [3].

The aim of the present work is the study of the phase stability of 3*d*-metal spinel ferrite powders placed into organic liquids in the presence of oleic acid. The spinel ferrite powders containing copper or cobalt cations were formed on the steel surface contacting with inorganic salt solutions in the open-air system when the rotation-corrosion dispergation (RCD) method was applied [4]. Oleic acid (38 – 40 wt. %) dissolved in *n*-hexane or chloroform was used for the preparing of organic media. The contact of a disperse phase with the dispersion medium lasted for 24 h. The X-ray diffraction (XRD) and X-ray fluorescence spectroscopy (XRFS) were chosen as the main methods of the investigation.

The copper-bearing samples were formed on the steel surface when it was contacting with $CuSO_4$ and $CuCl_2$ water solutions. The further contact of the spinel ferrite powders with organic liquids containing oleic acid resulted in color staining of the dispersion medium in dark green. The similar coloration was fixed for the samples heated in the temperature range from 80 to 740 °C. The obtained data can be related to the desorption of copper cations from the spinel ferrite's (magnetite) surface as well as from the surface of the products of its thermal transformation (maghemite or hematite) and the subsequent formation of green-colored $Cu[oleic]_4^{2-}$ complexes. According to XRFS data the organic media collected at the average ~ 95 mass. % copper and < 5 mass. % iron. The peak intensity of copper lines ranged from 1125 to 2300, whereas such parameter of iron did not exceeded 150-350. Hence, we may suppose that copper does not get included into the crystal lattice of iron-oxygen mineral phases and it is fixed only on their surface. According to XRD data the phase compositions of the initial powder formed in $CuSO_4$ solution and the same powder after contacting with oleic acid in *n*-hexane are similar, but in the second case the relative quantity of an oxyhydroxide part has insignificantly increased. Completely different chemical behavior was detected for cobalt-containing samples. The powders formed when the steel surface was contacting with cobalt sulfate solutions ($c[Co^{2+}] = 100$ mg / dm^3, pH = 6.5, and T= 50 °C) kept the phase stability in both organic liquids containing oleic acid. The result of XRFS observation points to the presence of "trace" quantity of iron and cobalt species in both organic liquids. Despite the fact that Co and Cu line's intensities are smaller than < 100, iron 75 – 90 wt. %, far exceeds cobalt, 10 – 25 wt. %. Such result confirms the phase stability of cobalt-bearing spinel ferrite powders in organic liquids containing oleic acid species. The obtained data permit to define the cation binding mechanisms that take place under the RCD conditions and confirm the difference in physical-chemical properties and catalytically activity of Cu and Co-bearing spinel ferrite nanoparticles [5].

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BIAS DEPENDENCE OF THE PHOTOCURRENT FORMATION IN A MOLECULAR DIODE

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We use the nonequilibrium density matrix approach to describe the photocurrent formation in the nano-device "electrode–molecule–electrode" (molecular diode). In the framework of HOMO–LUMO model the kinetic equations for charge transmitting processes were obtained. It was shown that in case of moderate-intensity light the photocurrent can appear in molecular photodiode even if no applied bias voltage. The direction of the light-induced current is determined by the asymmetry of coupling between the molecule and electrodes [1, 2].

It was shown that in case of such nano-device with an asymmetric coupling of the molecule to the attached electrodes, the tuning of photocurrent is made possible with alteration of transmission gaps by changing of biased voltage. Transmission gaps determine energy differences between the device's states associated with the charged and uncharged molecule. It is shown theoretically that the molecular diode is able to exhibit the photochromic effect (shift of illumination frequency). The effect is especially noticeable in the case of different space distribution of an electron density over the molecular orbitals [3].

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STUDY WITH ION BEAMS ANALYSIS OF THE ISOTOPIC COMPOSITION OF BC_4 OF RECEIVED CVD METHOD

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Preparation of ceramic samples of boron carbide by chemical vapor deposition (SVD) is to receive a sample with a homogeneous stoichiometric and isotopic composition. Changing the stoichiometric composition in the direction of increasing the boron concentration significantly affects the basic thermoelectric characteristics of boron carbide and the change in the isotopic composition of boron influences the radiation resistance, moreover if the material thermal converter branch used to convert thermal energy into electrical energy from nuclear reactors and isotope sources. However, it is of interest, especially in the process of development of the technology, to explore the real distribution of isotopes.

Boron isotope distribution was studied using nuclear reactions $^{10}B(p,\alpha\gamma)^{7}Be$ and $^{11}B(p,\gamma)^{12}C$, while in the best depth resolution was about 400 Å. When studying the distribution of carbon used in nuclear reactions $^{12}C(p,\gamma)^{13}N$ and $^{13}C(p,\gamma)^{14}N$, and in this case, the best resolution was equal to 470 Å.

The distribution of boron and carbon isotopes studied on a series of samples of boron carbide. For each of the samples of measurements were carried out with a certain way to change the energy of the incident protons. Proton beam current was equal to 1.5 – 2.0 μA. Each spectrum was measured to achieve the targets of the charge of protons in the 3000 μKl. Research results indicate that the ability to control the distribution of stability.

IDENTIFICATION OF TURBOSTRATIC BILAYER GREPHENE IN CARBON TRIBOLAYERS

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Carbon is liable to structural alterations under mechanical stress owing to its intrinsic sliced crystal structure with extremely weak bonds between basic layers. In nanoscale perspective, friction modifies the chemical bonds causing morphological and structural changes in carbon tribolayers (CTL), i.e. in graphite trace rubbed onto a substrate [1, 2]. Friction forces can impose pressure so high to break, disorient or distort chemical bonds in carbon tribolayers (CTL).

Optical response, Raman scattering and X-ray diffraction (XRD) of the CTL carry the fingerprints of sp^2-bonded carbon mono- and bilayer graphene together with those of diamond-like carbon structures. XRD takes place at $2\theta = 26.55\,^\circ$ emerging on the vague background. The layer spacing in CTL is found to be 0.357 nm which is higher than spacing in sp^2 crystals. Also, by Atomic Force Microscopy nanoscaled thin layers were found on the surface of CTL.

The Raman spectrum of CTL contains the feature of bilayer graphene-equal intensity of G and 2D peaks. D, G and 2D peaks are symmetrical and each peak fits to a single Lorentzian. We estimated that this lineshape comes from turbostratic bilayer graphene [3]. The assumption is supported by the wider spacing between graphene layers in the CTL [4].

The CTL with removed surface strata, exhibit altered physical behavior. The features related to crystalline sp^2 structure fades out in all experimental measurements. Namely, the peaks in Raman scattering and XRD quench, the optical absorption loses the feature of sp^2 structure. The residual carbon structure behaves like DLC with absorption above about 5 eV. Hence, optical absorption in as-obtained CTL results from overlapping of optical transitions due to both electron-hole coupling in sp^2 turbostratic bilayer graphene and DLC.

In sum, the CTL is morphologically anisotropic through the layer thickness and contains strata of different phases in a ordered through-thickness sequence. Mostly sp^3-bonded thicker layer of DLC is at the bottom and sp^2-bonded turbostratic bilayer graphene is on the top of CTL.

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INVERSION PHOTOCHROMIC HYBRID SPIROPYRAN – SP$_{THQ}$AZ

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The marriage of two photocromic molecules - spiropyran and azobenzene can lead to the birth of novel hybrid materials SP$_{THQ}$AZ (**Figure 1**) [1].

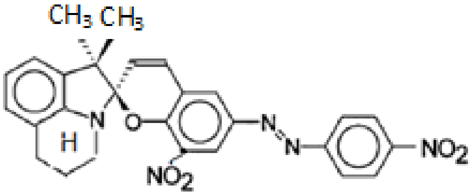

Figure 1. SP$_{THQ}$AZ.

The left fragment of hybrid molecule is indoline spiropyran modified by us with additional cyclic moiety which makes it rigid. Such compounds exhibits in polar solvents negative (inversion) photochromism. The colored MC form is more stable than the colorless SP form. In these cases, irradiation of visible light causes decoloration of MC to generate SP form. When SP form is placed in the dark, it returns to the colored MC form. Therefore, this thermally reversible photochromic system does not need the irradiation of UV light for its photochromism which may cause degradation of the compound. Studies have shown that such compounds are twice photosensitive to visible light than their indoline analogs. Due to the fact that thermodynamic equilibrium of the compounds with additional cyclic moiety in polar solutions is above photochemical - ($K_T>K_{PH}$) decoloration of system occurs with UV light too. The right side of the molecule - azobenzene extends π-conjugation system and causes bathochromic shift of the absorption band of the colored-zwitterionic form of SP$_{THQ}$AZ.

The molecule SP$_{THQ}$AZ combines the beneficial characteristics and properties of both components. Consequently photochromic properties can be controlled by lasers with different frequencies.

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NEW PHOTOCHROMIC HYBRID COMPOUNDS

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New hybrid compounds, which molecule contain two photochromic fragments of different nature have been synthesized and investigated. The marriage of photocromic spiropyran and azobenzene can lead to the birth of novel hybrid materials SPAZ. Two types of photochromic hybrid compounds were synthesized (**Figure 1**): by coupling azobenzene with (I) indoline spiropyran or (II) tetrahydroquinoline spiropyran with increased sensitivity to visible light [1].

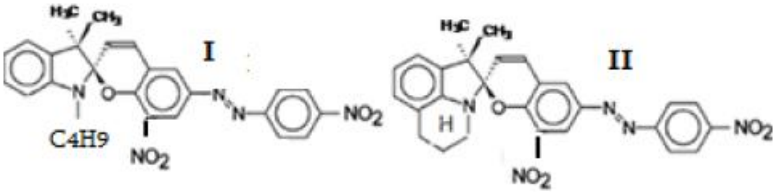

Figure 1. Two types of photochromic hybrid compounds synthesized.

Photochromic transformations and thermodynamic parameters were investigated (**Figure 2**) in the PMMA films dopped with hybrid molecules I and II at room temperature.

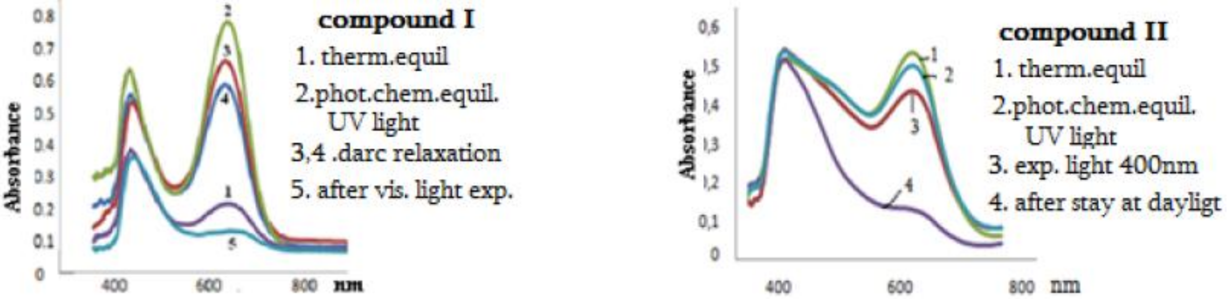

Figure 2. Photochromic transformations and thermodynamic parameters in PMMA films.

Bathochromic shift of the absorption bands, caused by elongation of the π-conjugation system, was observed in both types of samples. In sample II, in contrast to I [2], the thermodynamic equilibrium constant is greater than photochemical one and it is manifested in negative photochromism. In sample II, unlike I, due to the steric hindrance UV light does not affect the absorption band of the azobenzene moiety.

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NANOCOMPOSITE MAGNETIC MINERAL SORBENTS FOR SURFACTANTS REMOVAL FROM WASTEWATER

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The level of water pollution bysurfactants sharply increased in recent years. Most of surfactants and products of their decomposition are carcinogenic and toxic substances. Besides the efficient technology of anionic surfactants removal such as sodium dodecyl benzenesulfonate (SDBS) and sodium lauryl sulfate (SLS) are not elaborated [1]. Nowadays the using of natural sorption materials such as clays is a promising trend in water purification. It is caused by high sorption capacity, low cost and environmental susceptibility of this material.Inwater treatmentprocess the adsorption procedure are widely used in combination with magnetic separation.The modification of clay matrix by nanoscale magnetite is assumed.The use of magnetic composites prevents secondary pollution of water systems [2].

The aim of this work was to create effective and cheap sorbents for wastewater treatment from anionic surfactants.Synthesis was carried by impregnating matrix of saponite, spondyle and palygorskite clay bynanomagnetite in the form of magnetic fluid [2].Magnetic fluid was obtained by Elmore method. Samples of magnetic composite sorbent on the base of clay mineralswith various contents of Fe_3O_4 were received: 2 (MS–2), 4 (MS–4), 7 (MS–7), and 10 % (MS–10).

The magneticliquidwithanaveragesizeof Fe_3O_4 crystals 17.9 nm was obtained. Sorption capacity of nanosized magnetite relatively SDBS and SLS were 14.62 and 13.81 mg / g, respectively. As shown in **Table 1** the obtained nanocomposites have greater sorption properties with respect to SDBS and SLS in comparison with clays and magnetite.

Table 1. The maximum sorption capacity of sorbents relatively anionic surfactants.

	a, mg P / g				
Sample	Saponite	MS–2	MS–4	MS–7	MS–10
SDBS	8.14	31.91	35.16	36.24	23.27
SLS	5.19	28.67	30.24	35.60	24.87
Sample	Spondyle	MS-2	MS-4	MS-7	MS-10
SDBS	7.06	30.83	38.40	34.07	22.19
SLS	4.30	21.29	34.71	29.34	26.66
Sample	Palygorskite	MS-2	MS-4	MS-7	MS-10
SDBS	11.38	30.83	44.88	47.04	32.99
SLS	5.19	27.55	29.34	31.13	19.50

Through the presence ofmagnetite in an amount of 2 – 10 % wt. in the composites the maximum sorption capacity relatively anionic surfactants was increased in 2 – 5 times compared to the clay minerals. Moreover, the purification of water model solutions fromanionic surfactants by using clay minerals was lasted for 120 min. For samples of magnetic nanocomposites sorption equilibrium was reached in 60 min. This was caused bydevelopment of micropores and mesopores structure and formation of nanosized magnetite layer on the surface of the clay mineralspores. Creation of MS provided aggregative stability of nanosized magnetite. Hence the synergy effect was found.

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ELECTROMAGNETICS OF NANOCARBON STRUCTURES

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A great progress has been achieved during last two decade in the synthesis and fabrication of different nanostructured artificial materials with fascinating mechanical, electronic and optical properties irreducible to properties of bulk media. Accompanied by the impressive parallel development of the characterization techniques and measurement instrumentation, this process necessitates the revision of traditional concepts of physics and chemistry of condensed matter, adapting them to peculiarities of the nanoworld and significantly extending our knowledge of the nature of solids and our capabilities to control their properties.

Following this general trend, a research discipline – *nanoelectromagnetics* – is introduced as a synthesis of macroscopic electrodynamics and microscopic theory of electronic properties of different nanostructures. The approach is exemplified by carbon nanotubes (CNTs) and briefly touches upon other nanocarbon forms. Electromagnetic scattering theory is applied to calculate polarizabilities of finite-length single- and multi-walled carbon nanotubes (SW- and MWCNTs) in terahertz and IR ranges. Antenna properties of CNTs and CNT bundles are described. We demonstrate theoretically the dominant role of finite size effect in the non-Drude conductivity of CNT films due to the strong slowing down of surface polariton in CNT [1, 2]. The experimental evidence of the CNT length dependence of the THz spectra of SWCNT films [3] is presented. Thus, experimental results demonstrate the phenomena of localized plasmon resonance in SWCNTs and prove theoretically predicted antenna effect in SWCNTs in terahertz and far-infrared ranges. Significant screening effect is demonstrated to be inherent to electromagnetic response of MWCNTs films at gigahertz frequencies while it practically disappears in the THz range. The main features of the gigahertz and terahertz spectra of effective permittivity and electromagnetic interference shielding efficiencies of a MWCNT-based composite observed previously in experiments are systematized.

We demonstrate that surface plasmon–polariton waves with low phase velocity in carbon nanostructures can be utilized for the generation of coherent terahertz radiation through the Čerenkov mechanism [4], the effect being especially pronounced in spatially expanded double- and and multi-layer graphene structures [5].

We describe theoretically and demonstrate experimentally the anomalous absorption of microwave and THz radiation in graphene multi-layered structures [6] and pyrolytic graphite thin films [7] with the tens of nanometers thicknesses (much less than the skip depth). Theory predicts [8] that higher absorption can be achieved with a suitable choice of the dielectric permittivity and the thickness of the substrate.

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FUNCTIONALIZATION OF THE MULTIWALL CARBON NANOTUBES TO OBTAIN THE STRENGTHENING ADDITIVES FOR CONCRETE

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Carbon nanotubes (CNTs) have received considerable attention recently owing to their unique electronic and mechanical properties that are expected to lead to breakthrough industrial applications [1]. They can be synthesized by chemical vapor deposition (CVD), laser ablation and d.c. arc discharge [2]. Among these techniques, CVD has inherent advantages such as better control over process parameters and good scalability [3].

CNTs exhibit a well-known tendency to form agglomerates due to van der Waals forces, which makes them extremely difficult to disperse and align in a polymer matrix. The functionalization of CNTs is an effective way to prevent nanotube aggregation. It can improve their solubility as well as dispersion properties in solvents and in other systems. There are several approaches towards CNT functionalization including defect functionalization, covalent functionalization and non-covalent functionalization [4].

In this work the multiwall carbon nanotubes (MWCNTs) synthesized by Chemical Vapor Deposition over an Fe–Co / alumina catalyst were oxidized and grafted with maleic anhydride-1-heptene copolymer (MAH) via the “grafting to” approach using hexamethylenediamine bridge (HMDA). The obtained nanostructure was characterized by Raman spectroscopy, XRD, FTIR, SEM and TEM methods. FTIR confirmed the presence of the characteristic peaks of the anticipated zwitterion and amine-amide conversion. The completion of the grafting process was also confirmed by XRD and Raman spectroscopy. Microstructure images of the nanostructures obtained by TEM and SEM revealed that the MWCNTs are uniformly covered with the polymer which shows the effectiveness of the method. Whole the process proceeds at room conditions and that is the main advantage of this method [5 – 7].

The final nanostructure was used as the additive in preparation of the concrete samples and the mechanical properties of these samples were characterized by compression strength tester in comparison to initial samples. It has been revealed that the functionalization of the MWCNTs with MAH using HMDA makes them ideal additives for concrete.

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CARBON NANOTUBES: STABILITY, ELECTRO-KINETIC AND ADSORPTION PROPERTIES

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Carbon nanotubes (NTs) are promising materials for preparation of new type adsorbents, sensors and biosensors, catalyst supporters, composites, etc. In aqueous suspensions NTs have tendency for aggregation due to the strong van der Waals or hydrophobic attraction and they typically exist as large bundles and aggregates. Stabilization of aqueous suspension of NTs can be reached by adsorption of charge nanoparticles, surfactants or polymers, surface treatment.

In our study multi-walled carbon nanotubes were synthesized by Carbon Vapor Deposition method in the presence of Fe–Mo–Al catalyst. According to FTIR data their surface contained hydroxyl, carboxyl and carbonyl groups. Nanoplatelets of synthetic clay laponite RD ($Na^{+0.7}[(Si_8Mg_{5.5}Li_{0.3})O_{20}(OH)_4]^{-0.7}$) and surfactant cetyl-trimethyl ammonium bromide (CTAB) were used as the stabilizers of NTs in aqueous suspensions.

The experimental techniques included study of adsorption of dye methylene blue (MB) by nanoparticles in aqueous suspensions and measurement of the electro-kinetic potential of nanoparticles using ZetaSizer NS (Malvern). An increase in pH from 2 to 12 resulted in substantial increase of the absolute (negative) values of the ζ-potential due to the increase of dissociation of surface functional groups and the impact of pH on the positive surface charge at the edges of laponite. At neutral pH, the electro-kinetic potential of NTs and laponite reached –32 and –25 mV, correspondingly. Decoration of the NTs surface by laponite at mass ratios $X < 0.4$ ($X = m_L / m_{NT}$, g / g) caused a monotonic decrease in the negative value of the ζ-potential and at $X \geq 0.4$ its saturation was reached. This reflected the immobilization of laponite onto the NTs surface. Adsorption of CTAB resulted in overcharging the NTs and formation of a hydrophilic shell around nanotube.

The stability of NT suspension at addition of laponite and CTAB was investigated in a flow system using PDA 2000 Photometric Dispersion Analyzer (Rank Brothers Ltd, UK). The optimum ratio X (≥ 0.5) and concentration of CTAB ($C = 3.5 \cdot 10^{-5}$ M), corresponding to the maximum stability of suspension, were determined. A correlation between sedimentation stability of NTs suspension and ζ-potential of nanotubes was observed.

The kinetics of adsorption and parameters of equilibrium adsorption of MB on hybrid NT + laponite particles in aqueous suspensions at $X = 0 – 0.5$ have been investigated. Different stages on the time dependence of adsorption were explained by different types of interactions between MB and nanoparticles, changes in the structure of aggregates of NTs and long-term restructuring processes of laponite on the surface of NTs.

INVESTIGATION OF SURFACE PROPERTIES OF CHEMICAL VAPOR DEPOSITED AND TRIBOLOGICAL CARBON NANOSTRUCTURED FILMS

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Due to their unique properties, carbon nanofilms have become the object of general attention and intensive research [1]. In this case it plays a very important role to study surface properties of these films.It is also important to study processes of forming of this films, whichis accompanied by a process of self-organization at the nano and micro levels [2 – 4].

For more detailed investigation, we examined diamond-like carbon (DLC) layers deposited by chemical vapor deposition (CVD) method on Ge substrate and carbon tribo-layers obtained by rubbing [3 – 5]. In this report surface transformation of these CVD nanolayers is studied by atomic force microscopy(AFM) upon deposition time. Also, it can be successfully used to studysurface properties of carbon tribolayers. In turn, it is possible to sketch out their boundary line, which enables one to draw an idea of peculiarities of formation of these layers.

Images obtained by AFM are investigated as a mathematical set of numbers and fractal and roughness analysis were done. Fractal dimension, Regne's fractal coefficient, histogram, Fast Fourier transformation, etc. were obtained.The dependence of fractal parameters on the deposition durationfor CVD DLC films and on the number of sequential peeling for tribolayers was revealed. As an important surface parameter for our carbon films, surface energy was calculated as function of Regne's fractal coefficient [6]. Surface potential was also measured with Kelvin probe method using semi-contactingAFM. The dependence of surface potential on the deposition duration for CVD films and on the number of peeling for tribolayers was found as well.Results obtained by fractal analysis method was related with purely experimental results for number of samples.

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NEWCOMPOSITE COATINGS, THEIR STRUCTURE AND PROPERTIES

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The effect of structure and phase composition of composite coatings on their service properties under extreme working conditions (high temperatures and pressure, intensive wear by friction, external loads and corrosion environments) was considered. Here, the coatings of Ni–Cr–Si, WC–Co–Cr, Al_2O_3–Ti(Al), $ZrSiO_4$ systems and others, produced by applying the installation of a multi-chamber detonation of spraying, developed at the E. O. Paton Electric Welding Institute of the NAS of Ukraine, were investigated [1 – 3].

To make the detailed analysis of peculiarities of structural-phase state of the investigated coatings (microhardness, volume fraction of pores, phase composition, distribution of dispersed phases, nature of granular, subgranular and dislocation structures), the integrated investigations at all the structural levels were used, namely: optical metallography (Versamet–2, Japan; Leco–M400, USA), analytic scanning (SEM–515 of "PHILIPS" company, the Netherlands), as well as transmission microdiffraction electron microscopy (JEM–200CX, "JEOL" Company, with 200 kV accelerating voltage, Japan).

To evaluate the efficiency of the coatings being investigated under different service conditions, the analytical estimates of structure ↔ properties relations were used [4 – 7]. It was shown that the greatest contribution to the properties of strength, ductility and crack resistance of the investigated coatings were made by: dispersion of granular and subgranular structures, uniform distribution of forming strengthening phases of dispersed sizes in absence of lengthy and dense dislocation clusters, being the–concentrators of local internal stresses (potential zones of initiation and propagation of cracks).

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PERSPECTIVES ON THE ROLE OF NANOTECHNOLOGY IN SUSTAINABLE DEVELOPMENT

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Sustainable development is a comprehensive and complex system of systems requiring multidisciplinary and interdisciplinary science and technology inputs with economic, environment and social objectives. The trade space is very wide and the multitude of trade-offs generate considerable challenges and make it often difficult to achieve an effective balance In the last sixty years the planet's population has grown exponentially, from 2.5 to 7 billion people, andthe technological progress achieved has been tremendous. And they are expected to continue increasing even at faster rates. All these associated technological activities in the pursuit of better living standards have created considerable depletion of resources, pollution of land, water and air. Thus and because most of our resources are limited, it is imperative that we achieve more with less, or achieve higher efficiencies. This means that the amount of energy, water and other natural resources used in the production of a certain unit of goods, or in the achievement of a certain performance, must decreaseIn broad terms sustainable development is achieved when the present needs and challenges are met without placing in jeopardy the ability of future generations to meet their own needs and challenges.

Originally the nanotechnology agenda was dedicated to the discovery, modeling and characterization of nanoscale materials and phenomena. However, during the last ten years the focus has been on how nanotechnology can improve global sustainable development and develop itself in a sustainable mode.

The global energy demand is expected to increase by more than 50 % from now to 2025. The three main reserves of fossil fuels: oil, natural gas and coal are decreasing very rapidly and will not be always available to meet the global demands in the near future. The continuation of associated fossil fuel emissions will not be environmentally accepted, and there is a need to remediate some of the deleterious effects already sustained by the environment. Energy security has become a major and critical issue as fossil fuels are confined to a few areas in the world and their availability is controlled by political, economic and ecological factors. This means that in short term, considerable energy efficiencies and savings must be achieved, and alternative and renewable sources of energy must now be developed, with associated advances in energy storage and conversion materials and technologies such as batteries, super capacitors and fuel cells. The transportation industry accounts for one quarter of global energy use and has by far the largest share of global oil consumption. It used 51.5 % of the oil worldwide in 2003. Mobility projections show that it is expected to triple by 2050 with associated energy use. Nanoscale manufacturing can provide opportunities to consume less energy, less materials, less water and less manufacturing waste, and thus assist in the development of higher efficiency systems.

Considerable achievements have recently been obtained in the development of nano, nano-structured and nano-hybrid materials systems providing opportunities for industrial sustainability.

In addition component redesign using a materials and functional systems integration approach was used resulting in considerable system improvements and energy efficiency. This resulted in their introduction in the energy, transportation and manufacturing industries in a wide variety of devices and components with considerable technological, economic, environmental and social impacts. This presentation presents and discusses perspectives on the role of nanotechnology in sustainable development and focus of key areas such as energy, transportation, manufacturing, environment, water and climate.

B_4C–TiB_2 CERAMIC NANOCRYSTALLINE COMPOSITES: SYNTHESIS, COMPACTING, STRUCTURE, AND PROPERTIES

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In a single technological process, ceramic composite material B_4C–TiB_2 in nano-crystalline form is synthesized by the chemical synthesis method. For this purpose, there are used powders of amorphous metallic boron and titanium (IV) oxide, glycerol as a dispersion medium and at the same time as a carbon-containing reactant, and distilled water for achieving homogeneity of the mixture. Processing of liquid charge was performed in several stages by the thermal treatment at certain temperatures. Process proceeds under an inert atmosphere at temperatures up to 1300 °C. By varying the amount of precursors in the mixture, it is possible to adjust the ratio of the components in the final product.

X-ray phase analysis showed that the resulting black powder is a two-phase system consisting of boron carbide and titanium diboride. According to the electron microscopic studies, crystallites of the most part of powder mass have prismatic shapes and their size is less than ~ 100 nm.

Samples were compacted by the method of high-temperature compression and spark-plasma synthesis. Influence of technological parameters of the compaction on structure and physical-mechanical properties of compacted samples are studied.

PHOTOVOLTAIC PROPERTIES OF THIN FILM COMPOSITES BASED ON POLYVINYL ALCOHOL, OLIGOMERS OF N-GLYCIDYLCARBAZOLE AND THEIR HALOGENATED DERIVATIVES DOPED BY XANTHENE DYE

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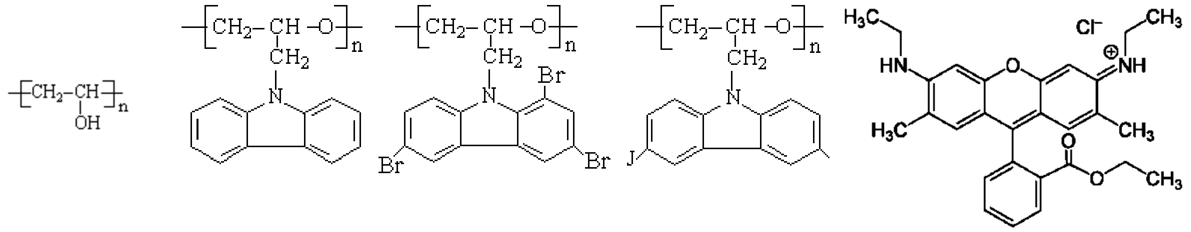
The photoconductive thin film composites (~ 1 μm) based on polyvinyl alcogol (PVA), oligo-N-glycidylcarbazole (o-GC), oligo(1,3,6-tribromo-9-glycidylcarbazole) (o-tri-BrGC), and oligo(3,6-diiodo-9-glycidylcarbazole) (o-di-IGC) doped with 10 mass. % of rhodamine 6G (R6G) have been prepared (**Figure 1**). The corresponding oligomers were synthesized by cationic polymerization method.



PVA o-GC o-tri-BrGC o-di-IGC R6G

Figure 1.

The photoelectric properties of these film composites were investigated by Kelvin dynamic probe method of surface electric potential measurement. It was shown, that all investigated film composites exhibit photovoltaic properties under illumination with light from the dye-sensitizer absorption region. It has been found that films of polymer composites based on polyvinyl alcohol doped with a xanthene dye possess photovoltaic properties, and the photovoltaic response varies little at the dye concentration greater than 10 wt % with respect to the weight of the polymer. The photovoltaic effect is caused by photogeneration of charge carriers in the dye aggregates and transport of non-equilibrium charge carriers among them. It is concluded that, in order to reduce the production cost of photoactive media for photovoltaic cells, it is possible to use cheap polymers with a low concentration of organic dyes. The reduction of photovoltaic response V_{PH} value in series o-GC- → o-tri-BrGC- → and o-di-IGC-based film composites was explained in terms of the heavy-atom effect on the non-equilibrium charge carriers photogeneration and transport processes. The spectral dependence of the observed effect was studied. The features of photoelectrical properties of obtained film composites, as well as the possible photodiffusional nature of the respective photovoltaic response are discussed. The respective phenomenological model for photovoltaic effect and internal photoeffect in investigated composite films is proposed.

SPECIAL FEATURES OF RADIATION EFFECTS IN NANO-DIMENSIONAL Si LAYERS AND IN Si-BASED STRUCTURES AND DEVICES

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It is well known, that from the middle of last century up to now Si is the main semiconductor of micro- (and now nano-) electronics. It is also well known that the problem of radiation immunity of semiconductor materials and devices plays one of the most important role in reliability of devices. The main physical basis of radiation influence on Si properties was developed and experimentally supported many years ago [1]. In compliance with these results the formation of radiation defects in Si is multistep process which includes some mechanisms of the point defects formation (vacancies – *V* and interstitials – *I* generation) and stable defects formation as a result of quasi-chemical reactions with the participation of *V*, *I*, atoms of donors, acceptors and background impurities and other defects of Si crystal lattice (including the surface). The concentration and properties of stable radiation defects in Si depend on irradiation nature and irradiation conditions. In electronics devices Si is a part of complicated construction which includes the layers of dielectric, metals, single crystal, amorphous and polycrystal Si. In many cases the irradiation changes of properties of multilayer systems and so changes the kinetics and properties of Si radiation defects because the electrical and elastic fields in such multilayer structures are sensitive to irradiation and so changes the radiation induced processes in Si.

In this report the peculiarities of radiation defects kinetics, spectrum and properties in Si nano-layers and nano-devices will be discussed. We will discuss not only problems which are condition of geometrical parameters of devices changing, but also the influence of new materials which are necessary to produce nano-devices.

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

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

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

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

As the aluminum concentration in composites increases the deuterium TDS is significantly changing and, as a result, the deuterium desorption temperature for $Al_{85}Ti_{15}$ composites sharply decreases ($T_m \sim 550$ K). A step-like shape of the maximum temperature curve of thermo-activated deuterium desorption, as a function of the component concentration change, evidences on the existence of two different structural states of the Al–Ti system depending on the ratio of components.

RETENTION OF DEUTERIUM INJECTED IN AUSTENITIC STAINLESS STEEL AT DIFFERENT IRRADIATION TEMPERATURES

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The samples of austenite 18Cr10NiTi stainless steel were studied. Deuterium introduction into the samples was performed by implantation of D_2^+ ions having the energy of 24 keV, current density of 2 – 5 μA / cm^2 with the doses ranging from $1 \cdot 10^{15}$ to $4 \cdot 10^{18}$ D / cm^2 at the sample temperatures 100, 240, 295, 380, 420 and 600 K. The ion-implanted deuterium desorption temperature variations as a function of deuterium dose. The sample structure was examined by means of transmission electron microscopy at a voltage of 100 kV. The X-ray diffraction analysis of the samples was performed with the diffractometer HZG–4 in the CuK_α-radiation (β-filter). The magnetic characteristics of 18Cr10NiTi steel and iron were measured with a bar-and-yoke permeameter. In this case the sample in the form of a plate was placed in the axial (perpendicular to its plane) field.

Deuterium thermal desorption spectra were investigated on the samples of austenitic stainless steel 18Cr10NiTi preimplanted at 100 K with deuterium ions in the dose range from $3 \cdot 10^{15}$ to $5 \cdot 10^{18}$ D / cm^2. The kinetics of structural transformation development in the implantation steel layer was traced from the spectra of deuterium thermal desorption as a function of implanted deuterium concentration. At saturation of austenitic stainless steel 18Cr10NiTi with deuterium by means of ion implantation, there occur structural-phase changes depending on the dose of implanted deuterium. The maximum attainable concentration of deuterium in steel is C=1 (at. D / at. met. = 1 / 1). The increase in deuterium concentration up to $C \leq 0.5$ leads to the formation of deuterium molecules inside the crystalline structure, in addition to the solid solution of deuterium in steel. Upon reaching the deuterium concentration of $C > 0.5$, the presence of these molecules causes shear martensitic structural transformations in the steel, which include the formation of characteristic bands, bcc crystal structure and the ferromagnetic phase. At $C \geq 0.5$, two hydride phases are formed in the steel, the decay temperatures of which are 240 and 275 K. The hydride phases are formed in the bcc structure resulting from the martensitic structural transformation in steel.

At temperature of 295 K, the TDS from steel show three temperature regions of deuterium desorption: (1) the peak with the maximum temperature $T_{\max}$ = 380 K (solid solution of deuterium in steel) with deuterium concentration of 2.5 to 3 at. % D; (2) the peak with $T_{\max}$ = 440 K and the retained deuterium concentration of 7 to 8 at. % D; (3) the region in a wide temperature range from 450 to 900 K with $T_{\max} \sim 500$ K.

At a temperature of 380 K, the TDS from steel exhibit a wide deuterium desorption region extending from 380 to 1200 K, with poorly resolved peaks having $T_{\max}$ ~500, 700 and 1050 K (local structure).

At temperatures of 420 and 600 K, the TDS show an extended region of deuterium desorption in the temperature range from the radiation temperature up to 1200 K, treated as being due to diffusion processes in the implantation layer. In this case, structureless regions are formed along the crystallite-local structure boundaries; steel components segregation also takes place.

PHOTOELECTRIC SPECTROSCOPY OF THE ELECTRONIC EXCITATIONS OF Si HETEROSTRUCTURES WITH NANOOBJECTS

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Semiconductor heterostructures with nanoscale objects attract significant attention due to the size quantization effects that lead to changes in the electron spectrum. The investigation of SiGe / Si heterostructures offers wide opportunities to develop new principles of nano- and optoelectronic devices such as medium and far infrared detectors, photodiodes, memory systems, lasers, etc. In Si / Ge heterostructures with Ge nanoclusters the spatial separation of nonequilibrium charge carriers takes place – holes in the valence band states are captured by Ge, and electrons are accumulated in the potential well of Si surrounding. As a result, Ge nanoclusters at low temperatures can accumulate positive charge. This determines the prospects of its application in novel nonvolatile memory devices [1 – 3].

We detected the local spatial distribution of the surface potential of the Ge NCs by using Kelvin probe force microscopy (KPFM) [4]. Different surface potentials between Ge NCs and the wetting layer (WL) surface were detected at room temperature.

The observed temporal evolution of the local contact potential differences (CPD) map confirms the ability of NCs to retain the holes during a long time after injection [5].

Also we are planning to investigate the properties of Si heterostructures with objects by using the method of photoelectric spectroscopy.

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METHANE MOLECULES IN α-NITROGEN MATRIX: STRUCTURAL STUDY

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Structure investigations of binary mixtures of the simple molecular crystals are of considerable interest. Solidified methane and nitrogen are the fundamental solids for solving problems of the solid state [1]. Moreover methane is known to occur in the planetary environments [2]. Solid N_2 are the formed by the linear and CH_4 – tetrahedral molecules. In the lattice CH_4 molecules demonstrate a tendency to approximate to spheres. Both the crystal have cubic (*fcc*) lattice at the equilibrium vapor pressure, symmetry of α-N_2 corresponds to the *Pa3* space group [3] and methane is described *Fm3c* [4] below 20.4 K. The nitrogen – methane solid phase diagram has been determined using X-ray diffraction method in studies [5, 6]. There are large discrepancies between results of these structural works. According to [5] a phase separation in CH_4–N_2 system was not observed and solutions are cubic at all temperatures below α–β transitions of α-N_2 at all concentrations. While authors [6] appointed that the mutual solubility of the components is practically absent in low temperature range despite the small difference in the lattice parameter of the components and their similarity of crystallographic structure. More experiments are required to resolve this controversy. Structure analyses of such solid solutions make it possible to obtain important information for a creation new theoretical approaches and a check of the existing models.

Structure of solid CH_4–N_2 mixtures was studied with the transmission electron diffraction techniques equipped with a helium cryostat. The samples were grown "*in situ*" by condensation gaseous mixtures on Al or C substrate at $T = 20$ and 5 K. The deposition regime was chosen in order to obtain random distributions of impurity. The error in the lattice parameter measurements was usually 0.1 %.

Based on analysis of the obtained diffraction patterns and the concentration dependences of the lattice parameter and diffraction intensity the region of existence of solid solutions was determined. The limiting solubility of CH_4 in the nitrogen matrix approaches 10 % mol. The phase separation of the solutions is studied. The effect of dilution CH_4 in N_2 molecular crystal matrix on the orientation order has been investigated. At low enough impurity fractions obtained data were analyzed with using cluster model.

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NANOTECHNOLOGY AND THE EFFECT ON PETROLEUM ENGINEERING EDUCATION AND RESEARCH

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Nanotechnology is an emerging technology with the potential to effect revolutionary changes in several aspects of the oil and gas industry such as exploration, drilling, production, enhanced oil recovery, refining and processing [1 – 4]. The importance of this emerging technology in petroleum industry presents a special challenge and opportunity to restructure teaching and nurture the scientific and workplace of the 21th century. This paper presents an overview of application of nanotechnology in the oil and gas industry to assess the importance and the potential technical benefits of this new emerging technology in petroleum industry. As a consequence of this rapid development and board impact of nanotechnology, education and training of new generation of engineering workplace, will play an important role in petroleum industry. In this regard, the effort to meet such demand while appropriately addressing and improving collaboration between the industry and academia, there is a strong need to introduce nanoscience technology into existing petroleum curriculum program. It is hoped that this work would be beneficial to both petroleum engineering education and research and will stimulate some idea for academics who may facedthemselves with the developing education course and teaching nanotechnology in the near future.

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THE EFFECT OF PARTICLE SIZE ON THE PHOTOCATALYTIC PROPERTIES OF TiO_2 POWDERS COATED WITH Co NANOCLUSTERS

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Photocatalysis decomposition of water into hydrogen and oxygen under the effect of sunlight is one of promising trends in finding the alternative energy sources. Water is not split by sunlight immediately. Currently titanium dioxide TiO_2 is acknowledged as a promising photocatalyst for this purpose [1]. In this substance electron-positron pairs, formed under the effect of solar rays on the photocatalyst surface interact with water molecules and split them into hydrogen and oxygen. Hence photocatalysts are used in the form of fine powders, to increase the surface area. Here comes a new problem: reaching the surface of a fine particle pairs undergo recombination very quickly. That is why it is necessary to coat the particles surfaces with nanoclusters which capture electrons or holes and hinder their recombination.

At E. Andronikashvili Institute of Physics, an original competitive method of deposition of nanoclusters of different substances on the surface of nanopowders was developed [2, 3]. The specific feature of the method is that the deposition proceeds at low temperature. Therefore, the method is simple and low-cost, it changes neither the properties of the matrix nor those of the material to be deposited.

By this method, Co nanoclusters were deposited on TiO_2 micro- (44 µm) and nano- (10 nm) powders. The experiments showed that, before deposition of nanoclusters on the particles surface, the light absorption by micropowders had been much higher than that of nanopowders, and that, after deposition of Co nanoclusters, the light absorption by micropowders increased slightly, while the absorption by nanopowders, coated with smaller nanoclasters, increased sharply, and, not only caught up with that by micropowders, but exceeded it. This indicates that in the nanoparticles more induced electron-positron pairs reach the surface than in the microparticles.

From the above discussion it can be concluded that the micropowders are unsuitable for photocatalysis, not only because they have a smaller specific surface area, but also because the specific efficiency of surface (efficiency per unit area) of nanopowders is much higher than that of micropowders.

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SYNTHESIS AND CHARACTERIZATION OF BIOPOLYMERS

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Chitosan is a biopolymer which is biodegradable in nature. Recently it is used in biomedical applications and has been blended with various macromolecules to mitigate undesirable properties.

The work deals with the synthesis and characterization of the Chitosan and Poly-ε-Caprolactone (PCL) solution – casted blended films in various proportions (Chitosan – PCL ratio 75 : 25 and 60 : 40). The casted films were subjected based on the structural, functional, optical and electrical studies by using XRD, FTIR, UV–Vis Spectrometer and LCR meter.

MULTISENSORY SYSTEMS BASED ON NANOSTRUCTURED METAL OXIDES

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Last time semiconductor gas sensors has become very popular due to their low cost, fast response time and good suitability to portable instruments. But in spite of these advantages, there is an urgent need to improve their "3S" parameters: Selectivity, Sensitivity and Stability [1, 2]. It is well known that sensitivity and stability of metal oxide gas sensors directly depend on structural characteristics of sensitive material such as morphology, particle size, surface-to-volume ratio, presence of additives, film porosity and film thickness. From this point of view, the most suitable are nanostructured materials, particular one-dimensional nanostructures, due to their high surface to volume ratio, and as a result, good values of the sensor signal [3]. Also 1D nanostructures have high chemical and thermal stability in different conditions and allow to create miniature and power-consuming microelectronic sensory devices on their basis. In this case, very important step is choosing of synthesis method and the process conditions.

More difficult task is improving of selectivity. There are several ways for increasing the selectivity of semiconductor gas sensors, including regulation of working temperature, usage of dopants and creating multisensory systems containing arrays of sensing elements [4]. As no one single sensor does not have 100 % selectivity to a single gas [5] and usually gives response of a number gases, it is very difficult to understand what caused the change in conductivity of the layer – gas type or it's concentration. That's why the last approach is very perspective because it allows to obtain distinct signal using a set of low-selective sensor elements. Usually multisensory system consists of several sensitive elements that differ in some way and have partial specificity. A particular gas interacts with a large array of different sensors. From each sensor comes a distinct response signal. Thereby, there is a possibility to obtain summary signal from several different elements – so-called chemical fingerprint for any particular component [6].

But in the development of multisensory systems researchers are faced with several problems. The first one is the criteria for selection of sensitive layers and their optimal number to create highly selective sensory element. Nowadays there is no clear selection algorithm of sensitive layer's type. It is also unknown how many layers will be need for creation of sensory element with sufficient selectivity. Other and not less important task is processing of the obtained data. For this, such sensory system must be equipped with good software that will work out sensory signals from all sensitive layers, consider the overlap sensitivity boundaries of different layers and form a total response for each component of gas mixture. Thus, creating of multisensory system will allow receiving a portable and highly selective gas sensor.

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INFLUENCE OF THE SHAPE OF MAGNETIC PARTICLES ON MAGNETO-OPTICAL PROPERTIES OF NANO-DISPERSIVE COBALT

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In the present paper, using the thin discontinuous Cobalt films as examples we have investigated the influence of the shape of magnetic particles on the magneto-optical and optical properties of the nano-dispersive structures.

In general, the magneto-optical properties of nano-dispersive magnetic structures are very different from the properties of the bulk ferromagnetic and depend on the structural parameters: the occupancy of the volume of the ultrafine medium with metal, the size and shape of the particles, the order of the particles, the properties of the medium, surrounding metal particles [1].

After generalization of the theory of effective medium approximation we arrived at formula how to calculate tensor componentsof the dielectric permittivity for non-spherical ultrafine particles [2]:

$$\varepsilon_{ef} = \varepsilon_0 \left(1 + \frac{q(\varepsilon_m - \varepsilon_0)}{y\varepsilon_m + (1-y)\varepsilon_0} \right),$$

$$\varepsilon_{ef}^{'} = \frac{\varepsilon_0^2 \varepsilon_m^{'}}{\left[y\varepsilon_m + (1-y)\varepsilon_0 \right]^2},$$

where $\varepsilon_m = \varepsilon_{1m} - i\varepsilon_{2m}$ and $\varepsilon_m^{'} = \varepsilon_{1m}^{'} - i\varepsilon_{2m}^{'}$ are the diagonal and nondiagonal tensor components of the dielectric permittivity of the material of magnetic colloidal particles, ε_0 is the dielectric permittivity of the non-magnetic phase, q is the volume fraction of the ferromagnetic particles and $y = f_2 - qf_1$, whilst f_1 and f_2 are the factors of the shape of the ultrafine particles and their surrounding medium. These formulas can be used to investigate which structural parameter has more influence on the optical and magneto-optical properties of the nano-dispersive cobalt. Obtained results have confirmed the significant change of the components of the tensor of effective dielectric permittivity and subsequently of the magneto-optical and optical properties which was brought about by the change of the shape of magnetic particles.

These calculations proved that if we take into account the shape of the particles, we will achieve a good agreement between the experimental results and the theoretical calculations.

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SILICATE COATINGS FOR HIGH–TEMPERATURE CORROSION PROTECTION OF STEEL IN OXIDATIVE ENVIRONMENT: PROCESSES AT SURFACE AND INTERFACE

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Oxidation of steel in atmosphere of combustion products limits its application in industrial practice. Once steel is exposed to oxidation conditions above ~ 570 °C, a multilayer scale constantly forms consisting of FeO (wustite) layer next to steel surface, Fe_3O_4 (magnetite) and Fe_2O_3 (haematite) at the scale-gas interface.

The aim of this work is to study the processes at surface and interface of silicate barrier coatings that prevent oxygen transport to steel surface and thus suppress it the progressive oxidation at elevated temperatures in contact with combustion products. The water-borne silicate composition was applied to Cold Rolled Steel (CRS) substrate. Almost complete curing of silicate coating by 650 °C was confirmed with FTIR and TG / DTG / DTA. SEM images (**Figure 1**) show that application of silicate composition (2.0 mol. Si / L) to bare CRS substrate (left) resulted in coating formation after subsequent curing at 650 °C for 0.5 h (right). The protective performance of the developed silicate coatings (**Figure 2**) was tested in air at 650 °C by substrates weight gain monitoring (**Figure 3**).

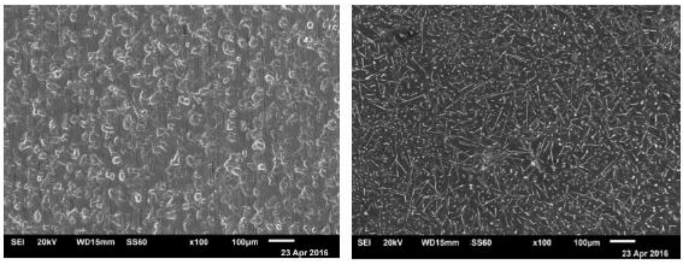

Figure 1.

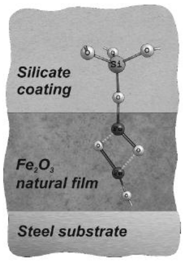

Figure 2.

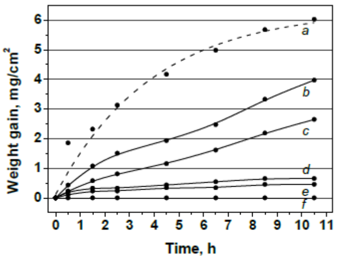

Figure 3.

The increase of silicate composition concentration resulted in enhancement of protective performance of 1- layer coatings while the best result exhibited 3-layer coating. The increase of composition concentration (*b* – 0.125, *c* – 0.25, *d* – 0.5 and *e* – 1.0 mol. Si / L) on CRS substrate resulted in enhancement of protective performance of 1-layer coatings. The best result exhibited 3-layer coating applied from 2.0 mol. Si / L composition – *f*. The formation of silicate coating on steel surface was simulated by *ab initio* Hartree-Fock method (within restricted open-shell variant) with valence-only basis set SBKJC and respective effective core potential using the GAMESS (Version 6.4) program package. Within 25 – 700 °C temperature interval, the calculated Gibbs energy for the reaction of silicate species bonding to Fe_2O_3 cluster appears to be close to – 270 kJ / mol ensuring the formation of Fe_2O_3 / Silicate interlayer responsible for adhesion and protective performance of barrier silicate coating.

The ongoing collaborative Project (2013 – 2016) “Production of Coatings for New Efficient and Clean Coal Power Plant Materials” (POEMA) is supported by FP7 Specific Programme “Nanosciences, Nanotechnologies, Materials and new Production Technologies” of the European Union.

DEVELOPMENT OF NANOTECHNOLOGY BASED BIOSENSORS FOR ENVIRONMENTAL MONITORING

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Bio-sensing and detecting biological and chemical organic substances in living cells are essential to many areas of life sciences, first of all to control the environmental ecological state. Modern cellular biosensors and biomarkers are very promising analytical tools for the environmental monitoring and effective bio-sensing of stress-induced reactions under dangerous environmental stress-factors. The application of nanotechnology based biosensors today has acquired a particular importance in connection with objectives of comprehensive science-based bio-monitoring.

Bio-monitoring stress-effects in plants, caused by the influence of biotic and abiotic environmental stress-factors, is critical for the effective environmental quality control. Use of stress-specific biosensors and biomarkers here is absolutely necessary for diagnostics of early stress reactions in plant cells. In this view, bio-sensing stress-induced cellular metabolites, most notably, reactive oxygen species (ROS) produced in cells under stress can be an efficient method of indication of important subcellular changes under harmful environmental conditions.

Based on the results of our current studies with a wide range of biosensors and biomarkers, we proposed a novel approach and nanotechnology-based strategy to the early stress sensing in cells that can be used the monitoring bio-objects at assessing of the ecological state and quality of regions. We propose to study and determine cellular mechanisms and signaling events underlying ROS metabolism in plants and animal cells during the stress response. The study will focus on different components of ROS scavenging system on cellular and subcellular levels. We intend to analyze ROS scavenging enzymes and low molecular weight antioxidants in cells and subcellular organelles: mitochondria, peroxisomes and chloroplasts in conditions of oxidative stress, caused by different environmental factors.

In our work, we applied the microwave whispering-gallery-mode (WGM) technique and nanowire field-effect electronic (FET) devices with microfluidic channels for characterization of molecular biomarkers and proteins as biosensors. It is expected that this approach will provide better sensitivity and increased selectivity of biomarkers sensing. The research foresees the measurement of characteristic responses of selected biomarkers and proteins in solutions at various concentrations and determination of ultimate parameters of the detection limit, quantification limit and dilution limit. In our experiments we tested several low molecular weight non-enzymatic antioxidants (ascorbate, glutathione) and antioxidant enzymes (superoxide dismutase, catalase) as samples. By systematic measurements, a set of characteristic responses of test substances at different concentrations and temperatures in the physiologically relevant aqueous solutions was obtained and analyzed. Experiments showed very good sensitivity and selectivity in detecting biomolecules at different resonance frequencies at the ng/ml level with high accuracy. The obtained results indicate the potential of our approach for non-invasive biosensing, as well as the prospect of new reliable nanotechnology-based biosensors for express-diagnosis of oxidative stress in living cells and environmental monitoring.

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MODIFICATION OF LOW ALLOYED CHROMIUM STEEL BY NANO-OXIDE COMPOSITE

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Medium-carbon chromium steel, which contains C 0.37 – 0.45, Mn 0.30 – 60, Si 1.20 – 1.60, Cr 1.30 – 1.60, S ≤ 0.035 and P ≤ 0.035, is applied in mechanical engineering for the production of high-strength and wear-resistant special-duty parts (shafts, fingers, rack-wheels, etc.).

In the development of nano-technology of modification highly-carbon-manganese austenitic steel by a nano-reagent, it's turned out that the effectiveness of the nano-particles impact essentially depends on the uniformity of their distribution in the metal [1, 2].

For the purpose of this, the briquettes containing iron and nano-Al_2O_3 were manufactured. Namely, a well-mixed powder of carbonyl iron (particles size of 160 – 200 μm) and nano-Al_2O_3 (nano-particles size of 30 – 100 nm) in the ratio of 5 : 1 briquetted by utilizing a double-acting 100-ton press.

Melting of the medium-carbon chromium steel was carried out in an induction furnace.
The study showed the positive effect of the modification by nano-Al_2O_3 on precipitation strengthening of medium-carbon chromium steel. It increases the hardness of steel after rolling or forging in average be 25.5 %.

Study of wear- stability was carried out on a rotary machine in conditions of dry friction. The studies did not include the impact-dynamic effect on the sample. Nevertheless, they are acceptable for comparative analyzes. Wear resistance of cast metal modified by nano-Al_2O_3 increases by 26 %.

The structure of both steel is ferrit-factured. It's clear that the steel modified by nano-Al_2O_3 is fine-grained in more extent.

By the electron microscopic (ultra-high-resolution FESEM for SE and BSE) examination of the rolled specimen it was found that nano-particles of Al_2O_3 existing in the steel structure are located in the boundary zones of the particles, where, presumably, intense diffusive processes (in two, three and higher orders of magnitude more intense than in the similar classic structure) take place. In result, grain boundaries are strengthened [3].

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LUMINESCENT PROPERTIES OF REDOX ACTIVE $Zr_{1-x}Ce_xO_2$ NANOPARTICLES

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Mixed cerium-zirconium oxides ($Zr_{1-x}Ce_xO_2$) has recently made a breakthrough in the field of development of three-way catalysts for automotive converters [1, 2]. As was shown in the number of papers, incorporation of zirconium ions into fluorite-type ceria structure leads to its local distortion accompanied by lowering of the energy of oxygen vacancy formation. This effect leads to both increased oxygen mobility and oxygen storage capacity (OSC) of the mixed cerium-zirconium oxide as compared to pure ceria.

While the excellent OSC properties of $Zr_{1-x}Ce_xO_2$ nanocrystals are widely accepted today, the content and arrangement of oxygen vacancies in these materials are still under discussion. In our previous papers [3, 4] using the methods of conventional luminescent spectroscopy we have determined the relative location of trivalent ions and oxygen vacancies for CeO_{2-x} and CeO_2:Eu^{3+} nanocrystals and the same techniques can be used for analysis of the processes of oxygen vacancies formation in $Zr_{1-x}Ce_xO_2$ nanocrystals.

In our work we have obtained nanocrystals $Ce_{1-x}Zr_xO_2$ with different zirconium concentrations (x = 0.1 and 0.2). We have shown that both increase of the concentration of zirconium ions, and transition from oxidizing to reducing atmosphere stimulates formation of additional oxygen vacancies in $Zr_{1-x}Ce_xO_2$ nanocrystals. Increase of the content of oxygen vacancies in $Ce_{1-x}Zr_xO_2$ is manifested in the higher intensity of the band formed by $5d \rightarrow 4f$ transitions of Ce^{3+} ions (390 nm) due to capture of the electrons remaining atoxygen removal by Ce^{4+} ions.

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DEFECTIVE NANOSTRUCTURE, INELASTIC PROPERTIES OF SiO_2, CaO AND AUTOMATED SYSTEM “KERN-DP” OF ANISOTROPY PROCESSING

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As is known, at annealing the impurity atoms start to migrate within the sample. As for the point structural defects, related internal friction (IF) maxima Q_{M}^{-1} are detectable, when the sample heating rate is $V = \Delta T/\Delta t = 0.1\,\mathrm{K/s}$. Assuming that the dissipation of the mechanical energy of elastic vibrations of SiO_2 + Si substrate is related to structural defects leads to the following expression for free-vibrations of a disc [1]:

$$\omega = \sqrt{\frac{D\beta^2}{\rho h R^4} - 2\pi^2\left(\frac{Q^{-1}}{T}\right)^2},$$

where substrate cylindrical rigidity,

$$D = \frac{Eh^3}{12(1-\mu)^2},$$

is determined via elasticity modulus E, substrate thickness h, and Poisson’s ratio μ. The β is the dimensionless coefficient dependent of the number of concentric circles, ρ is the substrate specific density, R is the substrate radius, Q^{-1} is the IF, T is the period of the vibrations of the disc. Elasticity modulus $E = 4.7\,\mathrm{kPa}$ and strength limit $\sigma_S = 4.2\,\mathrm{MPa}$ were determined for radiation-cross-linked hydrogel XX–6.

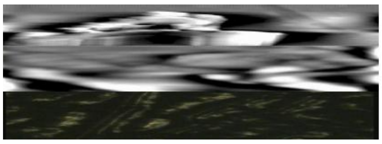

Figure 1. AFM porous microstructure of Si(100) surface ($15 \times 15 \times 10^3$ nm and $1 \times 1 \times 10^3$ nm).

Figure 2. Microstructure of $h \approx 200\,\mathrm{nm}$ thick $SiO_2+TiO_2+ZrO_2+Au_{0.03}$ film on Si(100) surface.

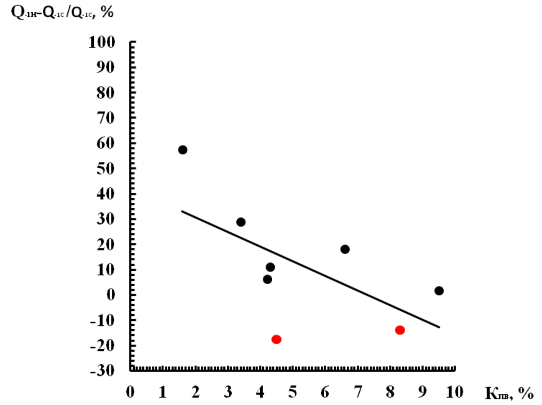

Figure 3. Correlative-dependence of SiO_2-defect internal friction $\Delta Q^{-1}/Q^{-1}$ from the open porosity ratio K_{PO}: 1 – before and 2 – after saturation.

Atomic force microscopy (AFM) microstructures of porous Si on Si(100) surface and $h \approx 200\,\mathrm{nm}$ thick $SiO_2+TiO_2+ZrO_2+Au_{0.03}$ film on Si(100), and correlative-dependence of SiO_2-defect internal friction $\Delta Q^{-1}/Q^{-1}$ from the open porosity ratio K_{PO} are shown in **Figures 1**, **2**, and **3**, respectively.

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OSCILLATING DEPENDENCE OF ELECTRON CONCENTRATION ON MEASURING TEMPERATURE IN IRRADIATED n-TYPE SILICON CRYSTALS

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It was investigated the change in the temperature-dependence of the electron concentration N in n-Si crystals irradiated at 300 K by protons with energy of 25 MeV with room temperature concentration of electrons of $6{\cdot}10^{13}$ cm^{-3}. The measurements were conducted by the Hall method in the temperature range of $T = 77 – 300$ K.

Annealing of the irradiated samples during 10 min at 110°C leads to the appearance of the $N(T)$ curve with two minima corresponding to the temperatures of 177 and 244 K. The observed oscillations of the electron concentration values can be explained by the electrostatic interaction between the charged point radiation defects – A- and E-centers, divacancies V_2, etc. – which appear around the nanoscale disordered regions with high (relative to the matrix) conductivity, so-called “metallic” inclusions, after a low-temperature (110°C) annealing of irradiated samples.

The electron energy at the local level is equal to $E = E_T + \varepsilon$, where E_T is the thermal energy, and ε is the average energy of electrostatic interaction between the charged defects around the “metallic” inclusions. With increasing in the crystal temperature, E_T grows monotonously, while ε depends on the degree of filling of A- and E-centers and divacancies V_2. However, these centers are charged from different temperatures. Accordingly, ε changes with the temperature step-wise. It is an explanation of the oscillatory dependence of the electron concentration from the measuring temperature.

PECULIARITIES OF CHANGES IN ELECTRON HALL MOBILITY IN DEPENDENCE OF MEASURING TEMPERATURE IN n-TYPE SILICON IRRADIATED WITH PROTONS

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There are investigated zone-melting n-Si crystals with room temperature electron concentration of $6 \cdot 10^{13}$ cm^{-3}. The samples were irradiated by protons with energy of 25 MeV at the temperature of 300 K. The Hall measurements were conducted in the temperature range 77-300 K.

Studies have shown that irradiation with protons leads to a sharp increase in the Hall mobility of electrons. This should be associated with the formation in a crystal in addition to point secondary radiation defects, nanoscale clusters of interstitial atoms with high relatively to matrix conductivity, so-called “metallic” inclusions.

The reducing in electron Hall mobility after annealing at 110°C is explained by the appearance of impurity-defect shells around “metallic” inclusions. After such a low-temperature heat treatment secondary radiation defects with low thermal stability, including a certain part of the E-centers, are annealed. Formed in this process non-equilibrium vacancies tend to the “metallic” inclusions of interstitial atoms and create around them a defective shell, which consists of A- and E-centers, divacancies V_2, etc. These defects are charged at different temperatures and thus “metallic” inclusion periodically – depending on the filling by electrons radiation defects and the electrostatic interaction forces between them – become “dielectric” (i.e., with low relatively to matrix conductivity) , i.e. opaque to electrons, what leads to the formation of the minima on the electron Hall mobility temperature-curve.

INVESTIGATION OF DIAMOND-LIKE CARBON FILMS AND PREPARATION OF CARBON NANOTUBES

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The morphology as well as optical and electrical properties of diamond-like carbon (DLC) films synthesized by plasma assisted chemical vapor deposition are described in [1]. Recently, structural changes in carbon films under external influence, the influence of hybridized states of carbon atoms, materials for doping the films for obtaining high conductivity and high carrier mobility as well as the dependence of refractive index on the technological parameters were studied [2 – 6].

In present report methods of nanotechnology controlling by means of measuring the spectra of plasma radiation depending on the gas composition and energy, affecting the cluster structure of obtained films in real time mode are discussed. Percolation capacities of clusters as well as conductivity of DLC differ in a wide range of cluster size.

Temperature dependence of conductivity testifies to their semiconducting properties. Here the results of measurements of spectra of optical transmission, reflection, photosensitivity and refractive index of obtained DLC films are presented. The AFM images of the surface of DLC films obtained for different content of initiators and parameters which effect the representation, morphology and histogram of obtained data. Surface nanotubes are seen with high resolution. Developed DLC films found different applications the list of which can be extended [7, 8]. Unique properties of these films improve each year.

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SYNTHESIS OF GOLD NANOPARTICLES FROM CHLOROAURIC ACID BY USING THE RED WINE

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Currently gold nanoparticles have found wide application in medicine and biophysical research. They are also promising for designing the devices of new generation. It is suggested by their unique properties. Unlike bulk gold, the gold nanoparticles possess ferromagnetic, catalytic and tunable optical properties. In particular, the optical properties of gold nano particles are determined by their plasmon resonance associated with the excitation of conduction electrons, and localized in a wide spectral region, from visible to infrared, depending on the size, shape and structure of nanoparticles [1]. The gold nanoparticles are chemically stable and biocompatible. Various physical and chemical methods are used for the synthesis of gold nanoparticles. However, these methods are expensive and involve the use of toxic reductants. Hence preference is given to alternative environment friendly methods of green chemistry.

In this work the process of production of gold nanoparticles from chloroauric acid ($HAuCl_4$) by using the red wine is discussed. The wine of two types was used: 1. The wine produced by ancient Georgian technology in qvevri (clay vessel) buried in the ground. 2. The wine produced in oak barrels. The synthesis was carried out at room temperature. The aqueous solution of $HAuCl_4$ of concentration 10^{-3} M was used. The wine was poured in small portions into the flask with the working solution. Saperavi wine was used simultaneously as a reductant and a stabilizer of the solution. The changed color of the solution pointed to the formation of nanoparticles in it.

The optical transmission spectra of the nanoparticles were studied with the help of UV spectrophotometer Sintra 10e. The absorption peak was recorded at 550 nm. The structure and sizes of nanoparticles were determined by using transmission microscope JEM–100SX. The size of nanoparticles varied over the range of 3 – 30 nm. The wine of both types was tested as a reductant.

It was revealed that the geometric shape of nanoparticles depended on the concentration of the working solution, and on the working solution–reductant concentration ratio. In diluted solutions, spheroid and ellipsoid nanoparticles were formed, while, with the excess of the reductant (wine), the nanoparticles of triangle, cubic and other geometric shape were formed. The histograms of size distribution of the nanoparticles were plotted and assessed.

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NUCLEATION OF SILICON DIOXIDE NANOPARTICLES IN THE FILM-FORMING TETRAETHOXYSILANE SOLUTION

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Nucleation of nanoparticles in liquid media is the first-order phase transition occurring in the metastable phase as a result of fluctuation formation of the nuclei of a new phase. The phenomenon of nucleation of nanoparticles has already found practical application in production processes, scientific research, medicine, biotechnology, etc. [1]. Silicon dioxide nanoparticles processing good biocompatibility are promising for target delivery of medicines.

This work deals with the nucleation of silicon dioxide nanoparticles in supersaturated solution of tetraethoxysilane (TEOS). Different TEOS solutions were prepared: one with ethanol, and another with a mixture of butyl and isopropyl alcohols as a solvent. Hydrochloric acid was used as a catalyst. The SiO_2 films were deposited on polished silicon substrates by centrifugation and were annealed stepwise in a thermostat up to 290 °C. The final annealing was performed in diffusion furnace KJ–1200–100IC at 450 °C for an hour with argon atmosphere. The relief of film surfaces was studied by using optical microscope LeitzErgolux with × 1250 magnification. The structure and size of formed silica nanoparticles were determined by transmission electron microscopy (JEM 100Sx).

It was revealed that, with the first solution, spheroid nanoparticles 5 – 50 nm in size were formed, while. With the second solution, there were formed nanoparticles of other shapes as well 10 – 70 nm in size.

The experiments showed that the factors such as the degree of supersaturation of the TEOS solution, the pH value of the medium, the viscosity of the sol and its temperature largely affected the processes of nucleation and obtaining of reproducible results. The size distribution of nanoparticles was determined and the corresponding histograms were plotted.

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SYNTHESIS OF MESOPOROUS SILICON DIOXIDE FILMS BASED ON SOL–GEL TECHNOLOGY

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Synthesis of new functional nanomaterials with specified parameters is one of main areas of nanotechnology. Recently the role of sol-gel technology for development of new materials and designing of new generation devices has considerably increased. In this connection mesoporous materials containing the pores with the diameters between 2 and 50 nm are quite promising [1]. Currently well-studied materials are the ones of type MSM–41 the frame of which has a regular comb structure. However, for production of the materials of this type, expensive and toxic substances are used. Hence the synthesis of mesoporous materials by using inexpensive and nontoxic materials is quite topical.

This work deals with the processes of deposition of mesoporous silicon dioxide films based on tetraethoxysilane (TEOS) and ethanol, and a template method. The films were formed on silicon substrates 60-100 mm in diameter by centrifugation at room temperature. After preliminary drying in a thermostat, final thermal annealing was performed in a diffusion furnace for an hour with argon atmosphere. The porosity of obtained layers was controlled by optical and transmission electron microscopy. The obtained films had a reproducible porous structure. The pores were of a cylindrical shape and 5 to 50 nm in diameter [2]. In the system of pores, mesopores dominated, while the proportion of macropores was quite small.

For production of mesoporous films by a template method, the same reagent (TEOS) was used as a source of silica-ions, and polyvinyl alcohol (PVA) was used as a template. The 1.5, 2.5, and 4.0 % solutions of PVA were prepared. The prepared solutions were mixed with TEOS in different proportions (1 : 0.5, 1 : 1, and 1 : 3). After deposition and drying in the thermostat, the samples were subjected to thermal annealing in the diffusion furnace at 550 °C with argon atmosphere. The experiments showed that the porosity of films increased with the increasing proportion of PVA, which is likely due to the increased specific surface area of the film. The porosity consisted mainly of mesopores, and the proportion of macropores was insignificant.

In the result of the investigation performed, the mesoporous silica films with cylindrical pores were formed. The obtained films can be used for the synthesis of new nanostructured materials and hybrid organic-inorganic films.

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STRUCTURAL PROPERTIES OF NANOSCALE MULTILAYERED TiN / ZrN COATINGS

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Vacuum arc deposition of a cathodes method (C–PVD) was used for deposition of multilayered coatings, based on nitrides of refractory metals, such as TiN / ZrN. Total thickness of the coatings was 11 – 19 μm, thickness of bilayers varied from 20 to 800 nm for different samples depending on different deposition conditions, such as bias potential, arc current, pressure of nitrogen in the deposition chamber. XRD, RBS, SEM, HR-TEM and STEM with local microanalysis, as well as nanoindentation were used for investigations of structure and properties of the mentioned above coatings.

RBS measurements showed, that in all layers of all coatings stoichiometric nitrides TiN, ZrN were formed with an average atomic concentrations 50 at. % (respectively to the type of coatings). Fabricated coatings demonstrated good mechanical properties, such as wear resistance and adhesion to the substrate, as well as quite high hardness.

STRUCTURAL, THERMAL, ELECTRICAL AND MORPHOLOGICAL CHARACTERIZATION OF $(Bi_2O_3)_{1-x-y}(Er_2O_3)_x(Tm_2O_3)_y$ NANOSTRUCTURES PREPARED BY SOLID STATE SYNTHESIS

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The solid oxide fuel cell (SOFC) is one of the most important in fuel cell technologies which produce electricity directly from gaseous fuel with an oxidant in an efficient and environmentally way. Although there are many researches about, yttria stabilized zirconia (YSZ) has been widely used as an electrolyte material in SOFCs [1]. However, YSZ requires high operating temperatures (1000 °C) [1, 2]. This high operating temperature causes many problems such as materials degradation, and requiring expensive noble metal electrodes. It becomes necessary to increase the operation temperature of the SOFCs to the intermediate temperature (IT) range (500 – 750°C) to have high ionic conductivity [3, 4]. Hence, decreasing the operation temperature is becoming a world trend to develop SOFCs [5 – 8].

In this study, erbium (III) oxide and thulium (III) oxide doped bismuth trioxide solid solutions, the $(Bi_2O_3)_{1-x-y}(Er_2O_3)_x(Tm_2O_3)_y$ ternary system were obtained with $x = 20$ mol. % and $y = 5$, 10, 15, and 20 mol. % dopant concentrations and $x = 5$, 10, 15, and 20 mol. % and $y = 20$ mol. % have been synthesized in air atmosphere and electrical conductivity properties of the samples have been investigated by 4-point probe technique seen in **Figure 1**. The crystal structure of the $(Bi_2O_3)_{1-x-y}(Er_2O_3)_x(Tm_2O_3)_y$ has been determined by X-ray powder diffractions (XRD) measurements before and after electrical conductivity measurements of the samples. Thermal behavior and thermal stability of the phases were investigated by differential thermal analysis (DTA).

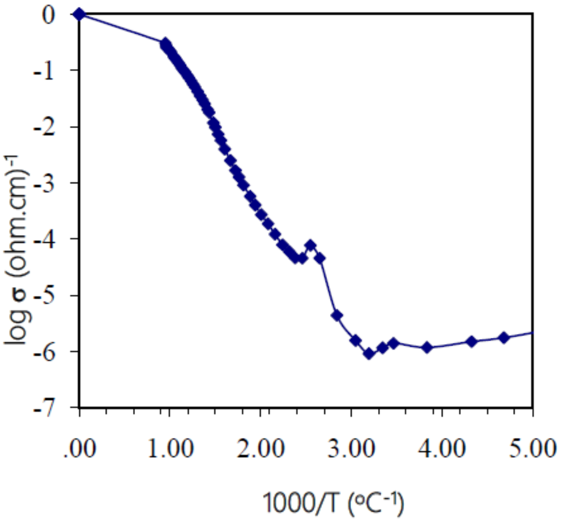

Figure 1. The temperature dependence of total electrical conductivity.

We investigated stable crystal structure at room temperature, electrical properties and possibility of stable cubic phase based samples containing $(Bi_2O_3)_{1-x-y}(Er_2O_3)_x(Tm_2O_3)_y$. Against this background, the purpose of present research is to determine the stable crystal ternary structures and an adequate dopant amount which has higher electrical conductivity, better stabilities over the wide temperature range and lower activation energy than the other samples. The samples which synthesized in this study can be used in diverse industrial applications such as electrolytes of the solid oxide fuel cells (SOFC).

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SILVER AND GOLD NANOPARTICLE DOPED POLYMER AND LIQUID CRYSTAL NANOCOMPOSITES FOR THE THERMO- AND PHOTO-OPTICAL APPLICATIONS

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In the last decade, gold and silver nanomaterials have received considerable attention due to their attractive electronic and chemical properties and their potential applications in the development of new technologies. Recent advances in the study of various gold and silver nanomaterials have led to their utilization in a number of very important applications including biosensing, diagnostic imaging, and cancer diagnosis and therapy [1]. The visualization and control of optical to thermal energy conversion in nano and microstructures is a key challenge in many fields of science with applications to areas as nanofluidics, nanocatalysis, photothermal cancer therapy, drug delivery, imaging and spectroscopy, information storage and processing, nanoscale patterning and solar energy harvesting [2, 3].

Here we report on the thermo and photo optical effects investigated in the silver and gold nanoparticle doped polymer and cholesteric liquid crystal nanocomposites. In particular:

1. Photo- thermal conversion in silver nanoparticles and thermochromic dye doped polymer nanocomposite.

In these experiments a polymer nanocomposite incorporated with silver nanoparticles and organic luminescence dye has been fabricated, which exhibits thermochromic properties. It was shown that this kind of composite dramatically changes its color when changes an environmental temperature and acts as a thermochromic material with such improved parameters as temperature controlled fine tuning of absorption and luminescence.

2. Light emission enhancement in cholesteric liquid crystal doped with luminescent dye and gold nanoparticles.

We have demonstrated that the light emission from a solution containing a luminescent dye can be enhanced when doped with a certain quantity of gold nanoparticles. When gold nanoparticles are added to a luminescent dye doped cholesteric liquid crystal mixture, we have observed a stronger luminescence and laser emission with respect to what was obtained using the pure mixture without gold nanoparticles. Obtained results can find versatile application in the field of fabrication nano sized storage media for quantum information devices, thermo controllable filters, windows and smart coatings, infrared image converters, for the visualization and monitoring of biological cells.

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PREPARATION OF NANOLAYERS BY LOW TEMPERATURE PLASMA ARC TECHNOLOGY

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In the present paper we are discussing the method based of usage of low temperature plasma arc technology for preparation of sub micro- and nanolayers of high-quality materials for different applications. The goal is to increase the adhesion in between the base material and sprayed layer, porosity reduction, increasing of density and receiving of predetermined other physical properties. These results are achieved by the fact that the sprayed material is heated, melted and evaporated then flows through accelerator nozzle and sprayed on base detail.

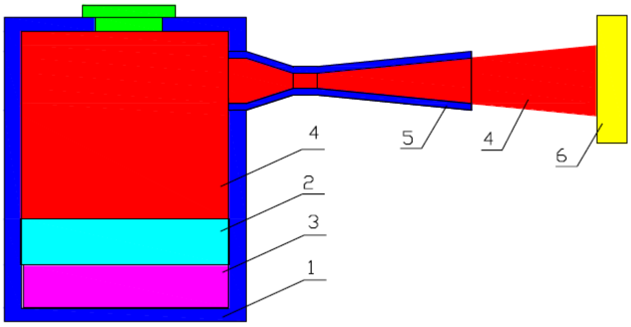

Figure 1. 1 – heat resistant container, 2 – material for spraying, 3 – heat source; 4 – steam of sprayed material, 5 – accelerator nozzle, and 6 – detail.

The heater that can be plasma arc is placed in a heat resistant container that melts and evaporates material that creates high pressure and flows through accelerator nozzle (**Figure** 1). Steam flow becomes supersonic in nozzle and then it will be sprayed on. Size of sprayed material and speed of hit depends on the distance between the detail and nozzle. It is especially important the combination of small size and high-speed which gives the opportunity to use the materials of different kind in sprayed layer. Also, by this method it is possible to receive mono or multi-component nano materials including the nano powders of industrial scale. It depends on type of the material placed in the vessel.

THEORETICAL DESIGN OF NOVEL NANOMATERIALS

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In recent years, intensive studies of the theoretical design of novel nanomaterials takes place, in which modern geometric methods are the key tool.

According to the Thurston's definition: n – dimensional geometry is a pair of $\Gamma = (X, G)$, where X – the differentiable n – dimensional Riemannian manifold in the $(n + 1)$-dimensional Euclidean space, G – maximum continuous topological group acting transitively on X in such a way that points stabilizers are the compact subgroups of group G.

In this paper, special attention is given to computer models and symmetrical aspects of two-dimensional and three-dimensional quasicrystals, namely the algorithms for constructing two-dimensional quasi-lattices whose point groups of symmetries belong to dihedrals groups D_m ($m = 8, 10, 12, 14, \ldots$) are developed. Visualization effect on such quasi-lattices of discrete subgroups of continuous topological groups is produced, and the corresponding quasiperiodic tilings of the Euclidean plane are made.

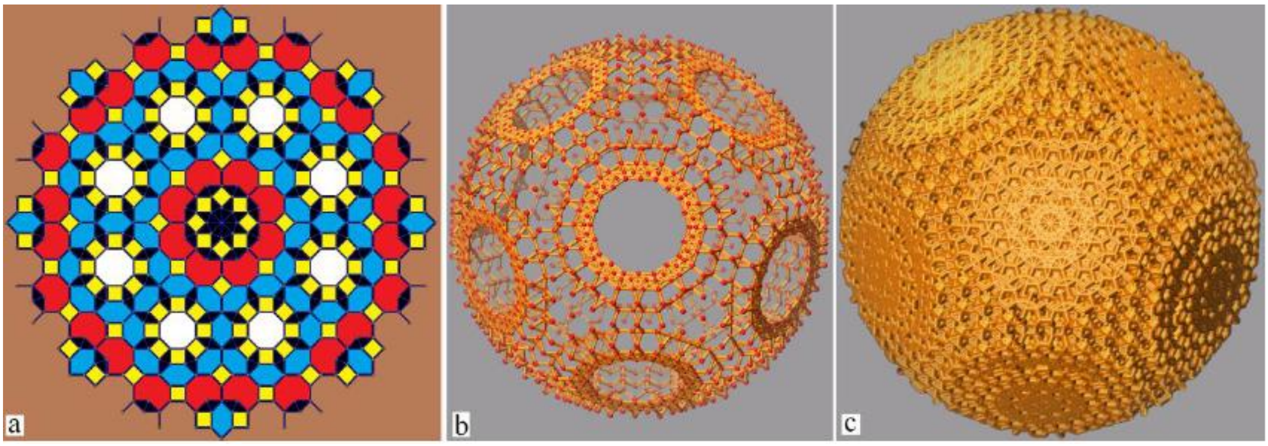

Figure 1. Projected crystals from multidimensional spaces on three-dimensional space.

By projecting crystals from multidimensional spaces on the three-dimensional Euclidean space, a variety of polyhedrons with non-empty interior, including full icosahedral group of symmetry I_h, are designed. The **Figures 1a**, **b** and **c**, respectively show as follows: (a) a fragment of tilings of the plane, namely: the dihedral symmetry group D_8; (b) the orthogonal projection of concentric spherical layer selected from a non-empty volume of a truncated icosidodecahedron, and (c) depicted in E^3.

The quantity of various tiles of quasiperiodic tiling shown in **Figure 1a** is equal to 5. The vertex angles of a triangle are as follows: 45, 67.5, and 67.5 ° (two such triangles make up a rhomb). The vertex angles of semiregular hexagon (hexagon is extended along the axis that passes through a center and two opposite vertexes) are equal to 90 and 135 °. The vertex angle of octagon is equal to 135°, and that of tetragon is equal to 135 °. 8 triangles converge to the critical point (the tiling center); triangles bases make up an octagon. Therefore, first coordination number of the critical point is equal to 8.

PECULIARITIES IN ATOMIC STRUCTURE OF NANOSIZED RHOMBIC TRIACONTAHEDRON-FACETED QUASICRYSTALS

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Since Shechtman's discovering quasicrystals in 1982 and winning Nobel Prize in Chemistry in 2011, the fundamentals of crystallography have been revised essentially.

In this work the models of an ideal nanosized quasicrystal such as rhombic triacontahedron with non-empty interior have been constructed by means of projecting from six-dimensional to three-dimensional space. The quantity of atoms in the said models is established to be discrete and correspond to the following sequence of integral numbers: 64, 729, 4096, 15625, ... The specified numbers can be obtained from the sequence of natural numbers beginning from number 2 which are raised to power 6. The quantity of model atoms can be determined by calculating and cubing the quantity of atoms on the external face or by calculating and raising to power 6 the quantity of atoms on the edge of polyhedron. The model of nanocrystal shown in **Figure 1** consists of 15625 atoms and belongs to complete icosahedral symmetry group I_h.

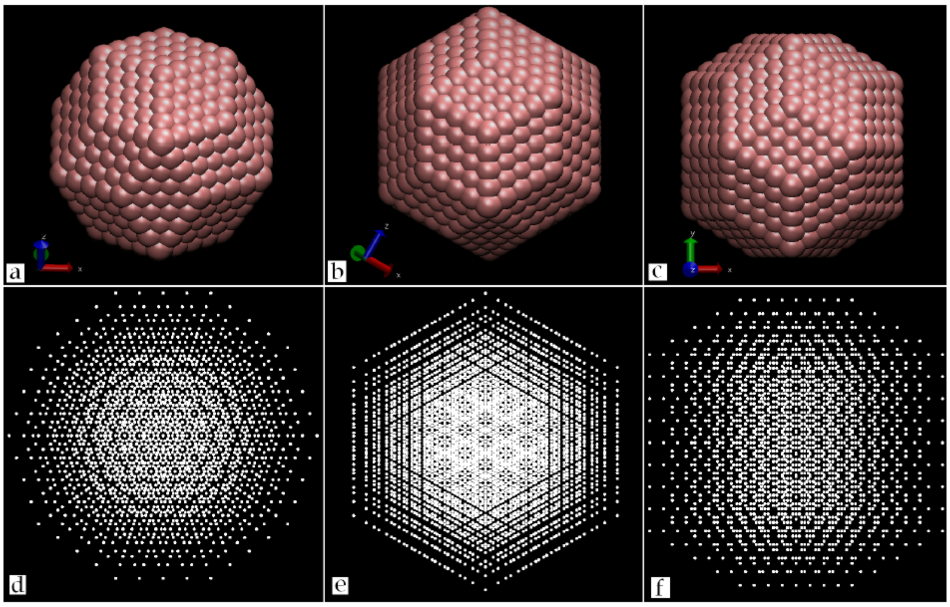

Figure 1. Rotary axes of 5-, 3-, and 2-fold symmetry of rhombic triacontahedron.

The model of the rhombic triacontahedron seen at three angles, and the rotary axes of 5-, 3-, and 2-fold symmetry are given in **Figures 1a**, **b**, and **c**, correspondingly. Fig. d,e,f presents orthogonal projections on the plane of model atoms set for a,b,c respectively. Such orthogonal projections are suggested to be similar to electron-diffraction patterns that can be obtained from the corresponding dual nanosized quasicrystal in the form of polyhedron, namely icosidodecahedron. A number of the features of atomic structure of surface layers of the said crystals are revealed.

SONOCATALYSIS FOR SILICA XEROGELS
USING IONIC LIQUID PORE TEMPLATE

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Two series of silica matrices have been prepared via acid catalyzed sol–gel processing; both classic and sonocatalyzed routes were used [1]. As silica precursors, tetramethoxysilan (TMOS) and methyl-trimethoxysilane (MTMS) were employed. In order to evaluate the influence of ionic liquid (IL) upon synthesis process and mainly upon silica material properties, a short chain ionic liquid, N-butyl-3-methylpyridiniumtetrafluoroborate([bmPy][BF_4]), was used in various IL / Si molar ratios in the silica precursors mixture. For both series of samples, the dry gels microstructure evolution with IL / Si molar ratios was explored by both small angle X-ray scattering (SAXS) and small angle neutron scattering (SANS) techniques (**Figure 1**) together with the nitrogen adsorption-desorption method.

Considering that the ionic liquid (IL) used as co-solvent can be catalyst and in the same time directing agent, this process is investigated in both classical and sonoactivated conditions. Results show that the ionic liquid played the role of catalyst that affected the formation of the primary xerogel particles, and also changed the porosity of the materials (**Figure 2**). The experiments show that ultrasound treatment resulted in a series of advantages. Sonogels, in comparison with xerogels, had increased pore diameter, larger pore volumes but diminished surface areas. The ultrasound treatment resulted in microstructure change on the level of the colloid particle aggregates. The pore size is almost double for sonogel samples with the highest studied IL content, compared to the non-sonicated xerogels. Thermogravimetric (**Figure 3**) and differential thermal analyses were performed for the $BMPyBF_4$ separately, as well as for the sonogels and xerogels with this ionic liquid. It has been shown that decomposition of the $BMPyBF_4$ in confined geometry starts at lower temperature compared to the pure ionic liquid.

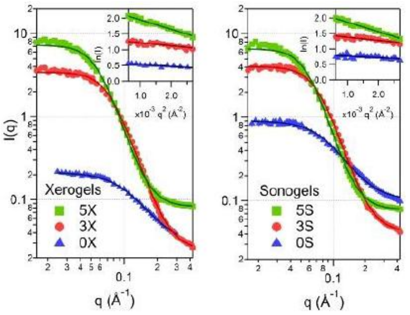

Figure 1. Small angle neutron scattering of IL templated xero and sonogels.

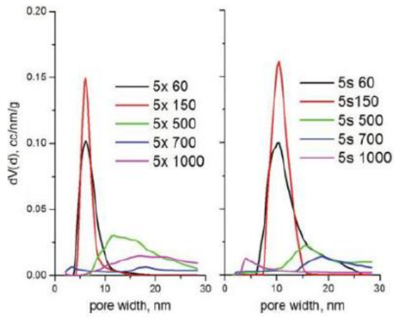

Figure 2. Pore size distributions of xerogels and sonogels with IL, in function of calcination temperature.

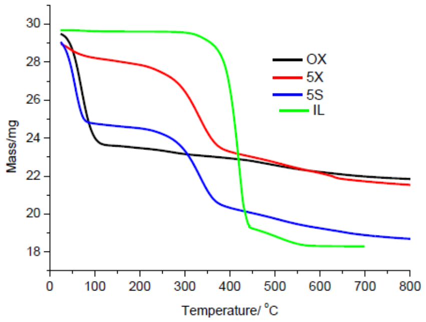

Figure 3. TG curves for TMOS / MTMS xerogel, xerogel with IL, sonogel with IL and pure ionic liquid.

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PHOTOTHERMAL EFFECT OF GOLD NANORODS AND OPTIMIZATION OF ITS STUDIES

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Photothermal therapy is a small-invasive method for tumor destruction by controlled thermal damage of tumor cells in the presence of photosensitizers or nanoparticles having a surface plasmon resonance, in particular, gold nanorods (GNRs). Parameters of plasmon resonance depend on GNRs properties, so search of the optimal needs many experiments.

We aimed at development of a protocol for analysis of GNPs photothermal effect on different models (tissue phantom, cell culture and animal tumor). We prepared GNRs with longitudinal plasmon resonance at a wavelength of 760 nm and 808 nm. GNPs were covered with linear polyethylene imine and were nontoxic for cells in culture. We used a continuous wave laser, 650 and 808 nm, with maximum power of 0.79 and 1.11 W / cm^2.

Tissue phantom (TF) is a non-cellular system resembling living substance for primary selection of laser irradiation parameters. TF allows reducing studies on cell cultures, which are much more expensive and laborious. We compared the effect of two lasers (650 and 808 nm) on TF at different laser power and time of exposure, and concentrations of GNRs from 0.01 to 0.4 mg / ml. TF allowed watch photothermal effect of GNRs and control the rate of heating. The level of heating depended on the content of the GNRs and the laser power. Application of a laser whose wavelength is closer to the maximum of GNRs plasmon resonance, leads to greater heating of TF. GNPs with longitudinal resonance of 840 nm and laser with a wavelength of 808 nm were used for studies on cell cultures.

Cultures of melanoma B16 cells and normal BHK–21 cells ($5 \cdot 10^4$ cells per well in 0.5 ml DMEM medium) were seeded on glass covers lips in 48-well culture plates, and incubated for 24 h. Then 0.1 μg / ml of GNRs in culture medium were added to cells and allowed to grow for 24 h. Irradiation of the cells for 15 min with laser (808 nm, size of a spot 5 mm) caused a damage of the cells only in the presence of GNRs. Decrease of spot size resulted in immediate cells death. Electron microscopy revealed that GNRs enter the cells and remain inside endosomes and lysosomes during the incubation before laser irradiation.

Melanoma in mice was generated by s.c. injection of $1.5 \cdot 10^5$ cells of melanoma B16 in 0.5 ml of sterile PBS to C57Bl/6 mice (18 – 20 g). The GNRs (0.2 μg / ml in 100 μL) were injected into tumors, which were subjected to laser irradiation after 48 h. The heating of a tumor was monitored with thermal imager, which detected heating of the tumors to 8.5 ° C larger in presence of GNRs. Mice were monitored for 4 days after irradiation and tumor sizes were measured, then mice were sacrificed and tumors were dissected for microscopy, which confirmed alteration of the tumors by photothermolysis. The differences in degree of melanoma damage by irradiating lasers (650 and 808 nm), related with different radiation ability to penetrate biological tissues were found.

Thus, optimal protocol for studies of GNRs photothermal effect includes subsequent use of TF, selection of the mode of laser exposure, experiments on cell cultures and in mice to demonstrate specific effect of the GNRs on tumor cells.

THIRD ORDER NONLNEAR OPTICAL SPIROPIRAN CONTAINING POLYMER SOLUTIONS AND LAYERS

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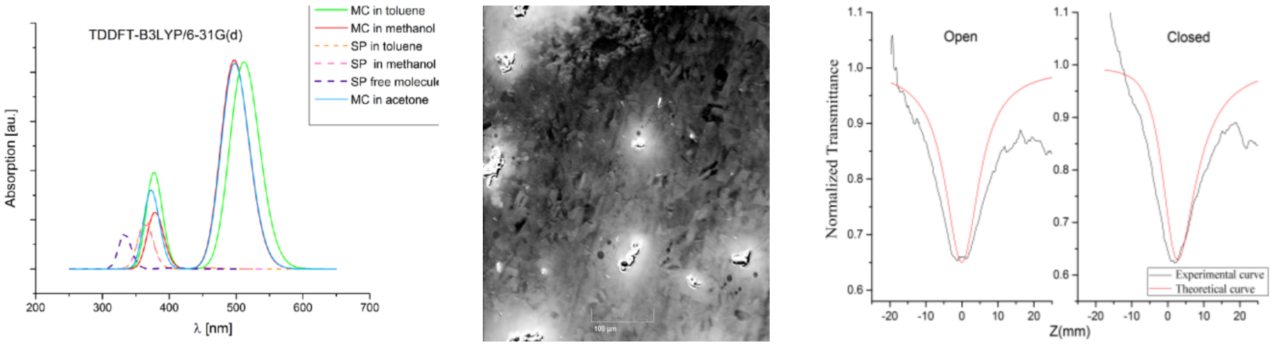
Transparent in visible region spyropirans (SP) undergo photochromic effect due to ultraviolet radiation changing to open form – merocyanine (MC). This may be the base to use them as molecular switches. As both SP and MC molecules generate strong NLO this switching may be seen also for second and third order processes. Nonlinear properties of both SP and MC molecules in polymer matrix were simulated within PCM model at DFT level using different functionals – namely B3LYP, Cam–B3LYP, LC–BLYP – and different basis sets. It occurred that polarizability and hyperpolarizabilites tensors values are several times greater than those calculated for urea which is often used as an reference.



Examples of absorption spectra of SP and MC in different solvents – spectra obtained from calculations.

Example of SEM picture of SP / PVA film with visible SP aggregates.

Example of SP in PS z-scan

Figure 1. Experimental evaluation based on z-scan measurements.

Experimental evaluation (**Figure 1**) is based on z-scan measurements. Data are collected for SP / MC solutions in mixture of polyvinyl alcohol (PVA) or polystyrene (PS) in tetrahydrofuran (THF). The same was done for layers of SP / PVA or SP / PS composites on quartz plates. Z-scan spectra were recorded both for open and for closed aperture leading to the possibility to calculate nonlinear absorption coefficient and nonlinear refraction index. Values of these parameters confirm pretty well that investigated materials have very good NLO properties. Samples with specific SP concentration reveal untypically strong effects both NLO and in absorption spectra. This was explained as a result of SP clustering within matrix, leading to occurrence of nanograins of this active species.

PREPARATION OF ULTRADISPERSE CRYSTALLITES OF MODIFIED NATURAL CLINOPTILOLITE WITH THE USE OF ULTRASOUND AND ITS APPLICATION AS A CATALYST IN THE ESTERIFICATION REACTION OF SALICYLIC ACID WITH METHANOL INTO METHYL SALICYLATE

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The acid modified natural clinoptilolite of Dzegvi (Georgia) deposit with different sizes of crystallites was investigated as a catalyst in the esterification reaction of salicylic acid (SA) with methanol (ME) for the synthesis of methyl salicylate (MS), which is widely used mainly in pharmaceuticals and perfume [1].

There was an effect of particle (grain) size – significant increase in catalytic activity of the simultaneously decationized and dealuminated form of the initial natural clinoptilolite (H-CL, νSiO_2 / νAI_2O_3 = 21.3, with detectable coarsely dispersed crystallites) with particle size reduction to ultrafine by ultrasound for 7 h (sample H-CL (UlS)) was observed.

For an ultrasonication the sample of H-CL in the form of water suspension (10% of water) was taken and it was processed ultrasound sequentially within 0.5, 1, 2, 5.5 and 7.5 h (Ultrasonic cleaner, DSA100–SK, 40 kHz, 100 W) [2]. After ultrasonic processing the distributions by the sizes of crystallites of catalysts H-CI (UlS) and H-CL on the laser light scattering particle size analyzer (Laser-Particle Sizer Analysette 12-DynaSizer, Fritsch) were determined; the dispersion medium was water [3].

The catalytic reaction of esterification was investigated in static system in conditions: temperatures 40 – 140 °C, molar ratios of SA/ME 1/3 – 1/10, the mass of the catalyst was 0.1 – 0.5 g; herewith for the more promising H-CL (UlS) catalyst the conversion of SA and selectivity of MS were the highest at a temperature of 120 °C and they are equal respectively, 90 and 95 % that considerably surpasses them for a H-CL catalyst with coarsely dispersed crystallites. The analysis of products of catalytic reactions was carried out by the GC-MS methods and UV spectroscopy.

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NEW APPROACH IN DEVELOPMENT OF DRUGS FOR MULTI-DRUG RESISTANT TUBERCULOSIS TREATMENT: METAL NANOPARTICLES EFFECTIVENESS

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Tuberculosis (TB) poses a significant threat to public health, in spite of all measures in the modern health care system. Annually active disease develops in 9 million people in the world, where in one third of patients disease is identified in a latent form. Every year an average of 2 million people die from the active TB despite of the existing treatment methods. Especially dangerous today is the wide spread of multidrug-resistant forms of tuberculosis. High level of multidrug-resistant TB threat and absence of current effective drug therapy provoke necessity in search of new approaches for development of drugs for TB treatment. Nanomaterials, especially metal nanoparticles, are possessed by good potential in this area due to their unique biological activity.

For the estimation of metal nanoparticles effectiveness as basis for development of drugs for multi-drug resistant TB treatment silver and copper nanoparticles have been synthesized by the method of chemical condensation by the reduction of their salts in water medium. Size, shape and chemical composition of nanoparticles have been characterized using TEM and energy-dispersive X-ray spectroscopy methods. Water dispersions of 30 nm spherical silver nanoparticles and 20 nm spherical copper nanoparticles have been synthesized. Mixture of silver and copper nanoparticles has been prepared with concentration of obtained substance 4.0 mg Ag and 32.0 mg Cu per 1 ml. Mixture of silver and copper nanoparticles has been studied for estimation of its tuberculocidal activity.

Tuberculocidal activity of the substance (Mixture of Ag and Cu nanoparticles) has been analyzed *in vitro* by Canetti proportion method using Löwenstein–Jensen medium. 10 resistant to isoniazid and 10 resistant to isoniazid and rifampicin clinical isolates of *M. tuberculosis* have been used for estimation of the substance's tuberculocidal activity. Total inhibition of growth for all analyzed clinical isolates of *M. tuberculosis* has been observed under presence of the substance in determination medium in concentration 0.08 mg Ag and 0.64 mg Cu per 1 ml.

At the same time the substance has been characterized as biosafe for eukaryotic cells using *in vitro* tests according to the parameters of cytotoxicity, genotoxicity and mutagenicity.

High tuberculocidal activity of the substance has been revealed *in vivo* under oral administration using model of guinea pigs' tuberculosis. *M. bovis* strain has been used for modeling of animals' disease.

The composition and technology of oral liquid dosage form has been developed using obtained substance in different concentration.

Obtained results indicate high perspectives of the synthesized nanoparticles in development of novel drugs for multi-drug resistant tuberculosis treatment.

CONTROLLED RELEASE OF DOXORUBICIN FROM MESOPOROUS SILICAS EQUIPPED WITH pH-RESPONSIVE MOLECULAR AND SUPRAMOLECULAR NANOVALVES

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In recent years, considerable efforts were made to move from sustained release systems to stimuli-controlled ones. The potential advantages of silica materials equipped with pH-sensitive pore-blocking structures for effective stimuli-responsive drug delivery were demonstrated in numerous works. Localization of pH-responsive blocking moieties near by pore orifices prevents preliminary delivery of encapsulated biologically active substance and contributes to its controlled liberation from mesopore volume in contact with the targeted cells. Various approaches were used for immobilization of pore-blocking structures at the construction of molecular [1 – 3] or supramolecular pH-responsive nanovalves [4 – 7] on the surface of silica carrier. Synthesized materials combine the unique features derived from a silica matrix and improved drug delivery ability.

In the present work, N-[N′-(N′-phenyl)-2-aminophenyl]-aminoalkyl groups, which serve as molecular pH-controlled nanovalves were designed on the external surface of MCM–41 silica by combination of sol–gel synthesis and postsynthetic modification. Supramolecular nanovalves were constructed from surface aromatic amino groups and β-cyclodextrin macromolecules supplied from a solution. Mesoporous structure of synthesized materials was characterized by low-temperature nitrogen adsorption-desorption, small-angle X-ray diffraction and transmission electron microscopy. Chemical immobilization of N-[N′-(N′-phenyl)-2-aminophenyl]-aminoalkyl groups was confirmed by IR spectral and chemical analysis of the silica surface layer. Loading and release behavior of synthesized drug carriers was studied in phosphate buffer solutions with pH 5.0 and pH 7.0 using doxorubicin as a test molecule. It was found that the loading efficiency of functionalized silica materials determined by UV spectroscopy measurements is 59 – 76 %, whereas cumulative values of Dox released from silicas with molecular and supramoleculars nanovalves into the phosphate buffer solution with pH 5.0 achieve 48 and 51 %, respectively. It was proved that silica carriers with aromatic amino groups and surface supramolecular structures localized near by pore orifices afford not only an abundance of silanol groups in the mesopore channels for effective loading of Dox molecules by the electrostatic interactions but also pH-controlled opening of pore entrances for pH-controlled release of drug.

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SILVER AND GOLD NANOPARTICLES: EFFICACY FOR TREATMENT OF MAXILLOFACIAL INJURIES AND THEIR COMPLICATIONS

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Oral and maxillofacial injuries, including facial bone fractures, are commonly widespread in the practice of emergency medicine and make up tangible percentage of the dental surgical patients. Such injuries are usually characterized by involving of combination of damages including soft tissues, bone, and teeth and often stay under high risk of the purulent-inflammatory complications. These factors provoke special attention to the applicable medications, which should combine antiseptic properties, anti-inflammatory activeness and stimulation of regeneration processes not only for soft tissues, but also for bone tissue. Among new created substances metal nanoparticles, especially silver and gold nanoparticles are possessed by high potential in this area.

Silver (AgNP), gold (AuNP) nanoparticles and their combination (Ag / AuNP) efficacy in treatment of maxillofacial injuries and their complications has been studied *in vivo* using model of *Wistar* rats' mandibular fracture with suppuration of the bone wounds and *ex vivo* using stromal stem cells isolated from the human bone marrow according to the method of stromal stem cells' cloning named after "Fridenshtein–Astakhova".

Water dispersions of sterile monodisperse spherical AgNP and AuNP with average size 30 nm have been used in this study. AgNP and AuNP have been synthesized according to the original protocol by the method of chemical condensation in water medium. Combination of Ag / AuNP has been received due to mixture of AgNP and AuNP in certain concentrations. Nanoparticles have been characterized as biosafe according to the parameters of cytotoxicity, genotoxicity, mutagenicity, biochemical markers (ATPase and LDHase activities) as well as LD_{50} parameter.

AgNP, AuNP and Ag/AuNP high antimicrobial and anti-inflammatory activity as well as stimulation of regeneration processes have been revealed according to the data of microbiological, histological and X-ray tests as result of *in vivo* experiments on the model of Wistar rats' mandibular fracture with complication. The data of *ex vivo* experiments according to the "Fridenshtein-Astakhova" method demonstrate that influence of AuNP and Ag / AuNP is characterized by stimulation of the clonogenic activity of the stromal stem cells at two times average in compare with control.

Obtained results indicate high efficacy of AgNP, AuNP and Ag / AuNP for treatment of maxillofacial injuries and their complications due to complex manifestation of antiseptic and anti-inflammatory activeness together with stimulation of regeneration processes.

PECULARITES OF RADIATION DEFECT FORMATION IN $Si–SiO_2$ STRUCTURES

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The energy spectrum and physical properties of low-dimensional nanoelectronic devices determined by the structure of the system itself and by a number of external (control) fields and impacts are well studied. However, the phenomena of influence of ionizing radiation and other penetrating exposures in these devices are still not understood. Any quantum, such as optical, for example, nanolasers, or information, for example, metal-oxide-semiconductor (MOS) structure system contains several metal-semiconductor, metal-insulator and insulator-semiconductor interfaces, at which external damaging impacts are rather different. Some of them, for example, space charges formed in dielectric layers, can be estimated by the Schrödinger equation, however an increase in the surface state (SS) density at the insulator-semiconductor (I-S) interface was studied insufficiently. At the same time the SS strongly affect the kinetics of physical processes in a system, reduce the carrier lifetime, increase noise, etc. The main part of the radiation defects introduced in semiconductor nanostructures is electrically active and forms energy levels that play an important role in the formation of electro-physical parameters of insulator–semiconductor (I–S) structures.

In present paper the comparative study of the parameters of radiation surface centres generated at the $Si–SiO_2$ interface after irradiation of MOS structure with different types of radiation has shown that, depending on the interaction mechanism between the bombarding particles and MOS structure atoms, radiation surface states of different nature are formed at the insulator-semiconductor interface. The energy spectra, annealing characteristic temperatures and the activation energies of the radiation interface centres depend significantly on the interaction mechanism. Electric fields, regardless of their sign, exert a significant influence on the formation of SS in the I–S system irradiated by fast electrons: they substantially increase the accumulation rate of radiation SS in $Si–SiO_2$ structures. It is interesting and important to note that the accumulation rate of radiation SS created in the $M-SiO_2–Si$ structures irradiated with fast electrons in the case of aluminium electrode is higher by a factor of 3 – 4 than that in the case of Au, Ag, Cu, Ni, Zn.

SHS METALLURGY OF CAST ALLOYS: STATE-OF-ART, CHALLENGES, AND RECENT ADVANCEMENTS

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Existing methods for production of cast alloys and related materials are normally energy-intensive and time-consuming multi-step processes. A promissory challenge is the preparation of cast alloys by using an energy-saving technique of self-propagating high-temperature synthesis (SHS) [1]. This technique has been originally developed in the 1960s and then used for synthesis of sintered refractory materials, high-purity ceramics, and intermetallics. Extensive studies of SHS reactions gave birth to the SHS technology for production of cast alloys [2] based on the use of thermite-type metallothermic reactions yielding intermetallics, carbides, borides, silicides, etc. Utmost advance was reached in fabrication of cast polymetallic alloys and intermetallics [3]. The above technology was also termed as SHS metallurgy [4].

The overall reaction scheme of the process can be represented as follows:

$$(Ox_1 + Ox_2 + Ox_3 + \ldots + Ox_n) + R \rightarrow [\text{polymetallic alloy}] + R_kO_l + Q,$$

where Ox_n stands for the oxides of Ni, Co, Ti, Cr, Nb, Mo, W, V, Mn, etc., R is metal reducer (Al, Ti, K, etc.), and Q – thermal effect of reaction.

Since vigorous metallothermic reactions are accompanied by splashing and loss of material, the process can be made much more effective when carried out in conditions of high artificial gravity[5] as in centrifugal machines. This affords to improve the yield of target product, facilitate the removal of gaseous products, diminish the grain size in the product, and make product more uniform (submicron and nano-size structural components).

A number of thus prepared multicomponent Ni, Co, Cr, Mo, Nb, Ti, Fe, etc. alloys, including a new class of so-called high-entropy alloys, will be discussed at presentation. SHS-produced cast alloys take advantage of their low production cost, fine-grained and uniform structure, and metallurgical heredity. Such alloys can find their application in aerospace industry, nuclear power engineering, implant surgery, etc. Implementation of metallothermic SHS can be expected to improve the quality of modern high alloys.

It will also be illustrated that our approach may turn suitable for deposition of cast protective coatings and for in-situ SHS surfacing. The coatings are formed due to strongly heat exchange between high-temperature alloys and substrate. The phase composition and microstructure of the deposited protective coatings will be overviewed at presentation.

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JOINT SYNTHESIS OF BORON AND TANTALUM UNDER CONCENTRATED LIGHT IN NITROGEN FLOW AND EFFECT OF TANTALUM DOPING OF BORON ON VIBRATION PROPERTIES

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Joint heatingfor powders of α-tetragonal boron with carbon impurities (~$B_{50}C_2$) and tantalum (Ta) in nitrogen flow in a xenon high-flux optical furnace was carried out at different conditions which is providing of light beam. As-received powder composed of h-BN, H_3BO_3, TaB_2, B_9H_{11} and a number of other phases including β-rhombohedral boron, apparently, heavily doped with Ta. FT–IR examination of any sample of the material reveals the complicated vibrational spectrum containing, in particular, an absorption band near 2260 cm^{-1}. The shapes of these bands are different for samples because powders were synthesized at different temperatures. Known, that in β-rhombohedral boron lattice, there are nano-sized voids of different types, which allows an accommodation of single atoms or small groups of atoms. Theoretical calculations performed by the method of quasi-classical type yields the same value, 2260 cm^{-1}, for the vibrations frequency of Ta atoms in D-type crystallographic voids in β-rhombohedral boron lattice. Since, Ta atoms are known to prefer accommodation just in D-voids, the experimentally detected bands can be identified with localized vibrations of Ta atoms.

PROPERTIES OF NANOSTRUCTURES AFTER EFFECT OF CONCENTRATED LIGHT

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Solar energy is a promising alternative energy source for nanotechnology because this energy is one of cleanest energy sources available. A xenon high-flux optical simulator (also artificial sun) that provides illumination approximating natural sunlight in controllable indoor tests under laboratoryconditions is a good model of this source. Optical simulator has numerous advantages. Its versatility, rapid heating and cooling rates, ability to adjust temperature profile along each axes, maximum operating temperatures and environmental adaptability stand out among others. Moreover, this technique can also be suitable for both conducting and non-conducting materials.

The results of study of the effect of concentrated light energy on transformation of boron nitride and boron powders with different additives named in [1] in a xenon high-flux optical furnace in a flow of nitrogen is presented. It isconsidered theheating under concentrated light energy, which lead to the formation of the melt, the process of boiling, evaporation of the melt, the formation of nanostructures in conditions of the corresponding temperature gradients and their deposition on the surrounding surfaces. Main driving force, which contributes to the formation and growth of nanostructures of different morphology,is analyzed. Properties of produced powders are presented and analysed.

Formation nanotubes, fullerene-like and graphene-like structuresis considered as a result of composition of initial powders and heating conditions.It is demonstrated that grain size of boron nitride powder produced direct synthesis of initial boron powders of different sizes*does not* have a direct correlation with grain size of the starting boron powder. The incorporation of the catalyst to boron powder provides a nanostructures and fibrous BN structures formation regardless starting powder grain size under proper conditions of temperature gradient distribution.

The presence of the OH group in nitrogen and additives of silicon, tantalum and indium in boron powder results in a change of chemical, phase and elemental composition, and also, the morphology of the obtained fine powders by increasing the number of nanostructured oxides and the new compounds in the phase composition of the material.

SEM and TEM investigations have shown preferential formation of two dimentional BN nanostructures along with equiaxed or plate nanostructures due to presence of H_2O during heating. “gaseous theory” which was developed for explanation of nanotubes formation and growth based on evolution of the bubble has found its confirmation in formation of two-dimensional BN nanostructures. Bursting of bubble, which easily formed in the presence of H_2O leads to this.

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ROS-SENSITIVE LUMINESCENCE OF CERIUM DIOXIDE NANOCRYSTALS

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Nanocrystals of cerium dioxide (nanoceria) due to their unique ability to spontaneous regeneration of antioxidant properties present nowadays one of the most perspective classes of redox-active materials for treatment of the negative consequences of an oxidative stress determined by action of reactive oxygen species (ROS) in a living cell. In our investigation we show that nanoceria beyond being effective ROS scavenger can act also as the ROS sensor allowing to determine ROS concentration in the cell. Moreover, using specific luminescent properties of nanoceria determined in our research, antioxidant characteristics of nanoceria can be easily controlled and its action in biological substances can be visualized by conventional spectroscopic techniques.

Our investigations involving both of UV–Vis and synchrotron radiation have shown that luminescence properties of nanoceria are determined by the presence and concentration of Ce^{3+} ions in nanoceria lattice. Content of Ce^{3+} ions is closely connected with concentration of oxygen vacancies and depends strongly on the size of nanocrystal and atmosphere of treatment. We have shown that at UV excitation intensive $5d \rightarrow 4f$ luminescence band of Ce^{3+} ions is observed in nanoceria at 390 nm. Nature of this band was confirmed by its excitation spectra obtained using synchrotron radiation which shows distinct five-fold splitting typical for f-d transitions.

Content of Ce^{3+} ions in CeO_2 determines also the antioxidant properties of this material, so intensity of Ce^{3+} luminescence can be used as a measure of antioxidant ability of ceria nanocrystals. Addition of hydrogen peroxide to nanoceria solution leads to fall of Ce^{3+} band intensity due to transfer of the part of Ce^{3+} ions to Ce^{4+} ones. The portion of Ce^{3+} ions underwent $Ce^{3+} \rightarrow Ce^{4+}$ transition increased with increase of the concentration of the oxidant – from 42 % at 0.1 mM to 70 % at 0.8 mM.

SYNTHESIS OF ORGANICALLY MODIFIED SILICA NANOPARTICLE / EPOXY ACRYLATE HYBRID RESIN

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The modification of silica nanoparticles by alkoxy silane coupling agents possibly leading in inadequate and varietyof concentration of functional groups were aimed to preventby using effective toluene diisocyanate (TDI) molecule instead of seemingly effective alkoxy silane coupling agents [1]. Well defined spherical, monodispersed silica nanoparticles (SNPs) were prepared by the sol–gel process based on the *Stöber method [2].*Surface modification of SNPs was achieved obtaining Si-TDI nanoparticles in order to gain both improved dispersion of SNPs in organic phase and ability for further possible reactions over free m- isocyanate groups of TDI.

Well defined Si–TDI nanoparticles were incorporated into synthesized Bisphenol-A type epoxy-acrylate (EA) resin over the urethane bond formed between hydroxyl groups of EA resin and free isocyanategroups of Si–TDI nanoparticle creating inorganic crosslinking pointsas illustrated in **Figure 1**. The curing process of SNP / EA hybrid resin was performed under UV irradiation and rheological,thermal and mechanical properties of the cured nano-hybrid resin were investigated.

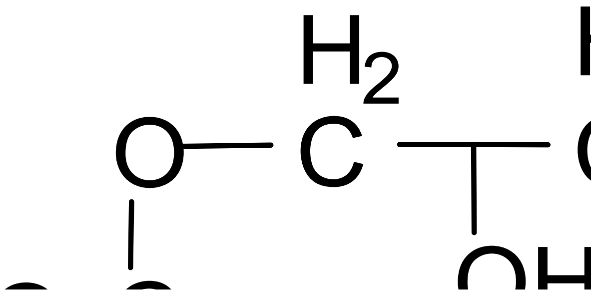

Figure 1. Silica nanoparticle / epoxy acrylate hybrid resin.

The results evaluated from SEM, tensile tests, DSC and TGA analysis were confirmed the crosslinker effect and monodispersity of Si–TDI nanoparticles which significantly improved the mechanical and thermal properties of UV-cured hybrid resins in addition to benefits of being an inorganic nanoparticle content [3].

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SURFACE AND CORROSION STUDY ON ELECTROREDUCED GRAPHENE OXIDE NANOSHEETS-COATED CARBON STEEL IN NaCl 3.5 %

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Electrochemical reduction of graphene oxide on a carbon steel electrode leads to the formation of reduced graphene oxide nanosheets (RGON). The samples were characterized using FT-IR, Raman, XRD, EDXA, SEM and TEM techniques. The anticorrosion properties were proven by electrochemical methods such as open circuit potential (OCP), potentiodynamic polarization (Tafel) and electrochemical impedance spectroscopy (EIS) in NaCl 3.5 %. Moreover, parameters affecting film formation and consequently anti-corrosion performance, such as deposition time and applied voltage, were optimized.

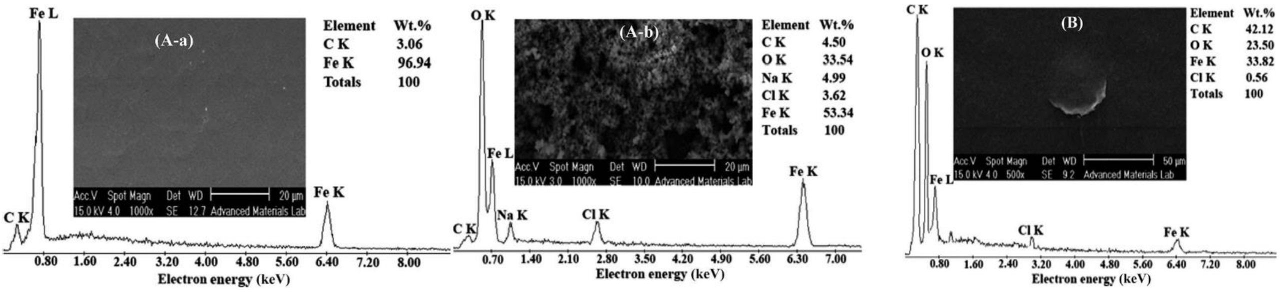

Figure 1. SEM–EDX analysis of; (A) the bare steel before (A–a) and after (A–b) exposing to 3.5 % NaCl solution, and (B) the RGON-coated carbon steel after immersion in 3.5 % NaCl solution.

Results showed (**Figure 1**) that covering the surface with RGON led to hinder the corrosion reaction (negative shift in the corrosion potential, a decrease in the slope of the cathodic and anodic reactions, a decrease in current density and corrosion rate, and an increase in charge transfer resistance). After applying 12 V during 180 s, the formed layer showed the best corrosion protection (the lowest corrosion current density and corrosion rate, and the highest charge transfer resistance). The morphology of the uncoated and coated surface after 72 h immersion in NaCl 3.5 %, was studied using SEM and EDXA techniques [1 – 3].

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Ni NANOTUBES: INFLUENCE OF DEPOSITION PARAMETERS ON STRUCTURE AND MAGNETIC PROPERTIES

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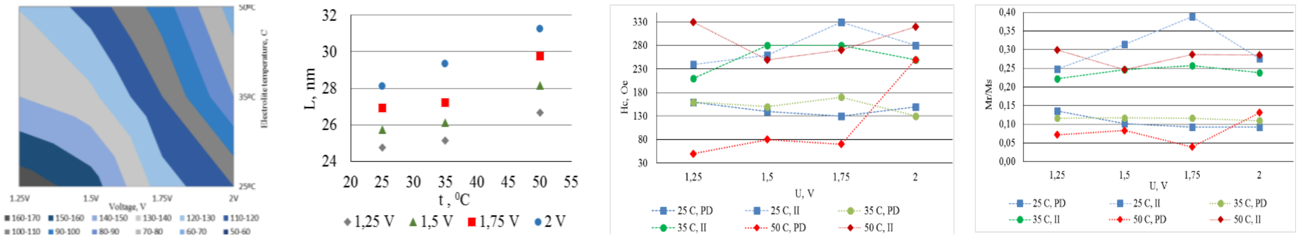
The most common methodof metallic nanotubes (NTs) synthesis is electrodeposition into pores of aluminum oxide template [1, 2]. However, the use of rigid substrates imposes some restrictions on the practical application.In our work the ability of flexible polyethyleneterephthalate ion-track membranes as templates for Ni NTssynthesis areconsidered.To understand the influence of deposition conditions (temperature, pH, voltage, time of process, pours diameter, etc.) on Ni NTs crystallinity and they morphologyseries of electrodeposition experiments of nickel were held on by SEM, TEM, SAED, EDA and vibrating magnetometry methods. Deposition potential as well astemperatureof a process leads to increasing of lattice parameter and decreasing of wall thicknesses. Magnetic properties also change under influence of deposition conditions. Results of morphology and magnetic propertiesinvestigations of series of experiments of pure Ni are shown on **Figure 1**.

Control of deposition parameters gives an opportunity to synthesize NTs with tailored parameters such as dimensions, crystallinity and magnetic properties.It could be noted, that metal nanotubes are considered very promising for high performance catalysts, highly sensitive gas sensors,nanoscale electronic and magnetic devices.



a b c d

Figure 1. Ni nanotubes, series of experiment 400 nm: (a) dependence of wall thickness (nm), (b) latice parametr, (c) coercitivity and (d) squarness of voltage and electrolite temperature.

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STUDY THE PHYSICAL PROPERTIES OF SOME METALS' AND SEMIMETALS' NANOCOMPOSITES

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Theoretically and experimentally approved that atoms, placed on the surface of chemical elements' nanoparticles, enhance sensibility in regards to atoms (molecules) of medium. Until today are less studied the physical-chemical properties of nanoparticles, which contain composites from two or some chemical elements and the influence on them of environment (disperse medium), temperature, magnetic field, aggregate state, etc.

The goal of work was to study the magnetic and electric properties of Pr^{3+} ($4F^2$), Gd^{3+} ($4f^7$), Dy^{3+} ($4F^9$) elements with magnetic moments, equal to $\mu_{eff} = 3.5$, 7.9 and10.5 accordingly, diamagnetic bismuth, antimony and carbon's multi-dimension nanosystems, carefully purified from gas oxygen and placed in medium ofliquid and solid diamagnetic water and different organic compound.

In research were used Kvinke'sviscosimetric and electro conductivity methods. Experiments were carried outin temperature interval 200 – 298 K. At using the viscosemetric method the increasing offluidity of studied systemswas provided by adding the organic substance on composite.The excitation of nanoparticles wascarried out by using the cavities of different size, i.e. by using the Kraunethers with different circles of ether oxygen.

Received experimental evidence shows, that abnormal character of changes of physical properties the searching systems significantly depends on chemical nature of components and aggregate state of medium. Temperature influence is not exhibited so strongly.

During studying of the nanocompisites' physical properties for explanation of some abnormal properties, which were detected, is offered the probable mechanism of process, which was induced by changes.

THE CATALYTIC PROPERTIES OF PHOSPHOMOLYBDIC ACID ATTACHED TO THE SURFACE OF AMINE-CONTAINING SILICA

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Heteropolyacids (HPA) are known as redox and acid-base catalysts. The phosphomolybdic (PMA) and phosphotungstic (PTA) acids with imbedded transition metals are among the most widespread ones [1, 2]. However, a significant disadvantage of these catalysts is their solubility in the reaction medium. Therefore, the task of finding carriers for these active centers is of current interest. Such carriers should endow the synthesized materials with thermal and hydrolytic stability, expand the sphere of their application due to the heterogeneity and retain functionality due to the porous structure. This work presents the catalytic properties of PMA supported on the amine-containing SBA–15 type mesoporous silica (synthesized by direct template method described in [3], but with different concentrations of ammonium groups). Two systems, differing in the nature of catalysis, were chosen as model catalytic reactions: cyclooctane oxidation and ethanol dehydration. The attachment of HPA was carried out from their concentrated aqueous solutions, wherein the blocking of carrier's pores was not observed. The resulting catalysts were examined by a number of physical and chemical methods such as X-ray, UV, IR, and NMR spectroscopies, nitrogen adsorption, TEM, SEM. It was determined, that catalytic properties of such materials are slightly worse compared with the free acid (**Table 1**). However, it was expected, considering the fact that in the later case the reaction is catalyzed homogeneously, and in the former – heterogeneously, and the number of active sites is much smaller.

Table 1. Catalytic properties of catalysts with attached PMA.

Samples	Oxidation of cyclooctane		Dehydratation of ethanol	
	Conversion, %	Cyclooctanone / cyclooctanole, %	Conversion, %	Ethanol / aldehyde, %
FMA	10.8	9.2 / 1.6	100	100 / 0.0
Catalyst 1	5.9	3.7 / 2.2	71.6	48.2 / 23.4
Catalyst 2	5.3	3.4 / 1.9	85.8	61.3 / 24.5

Our studies have shown that such carriers are promising for more complicated systems of HPA. Furthermore, HPA attachment is limited by the surface area of amine-containing materials. The synthesized catalysts may be used in a wide variety of catalytic processes.

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USAGE OF INTELLIGENT DATA PROCESSING FOR NANOMATERIALS STRUCTURE ANALYSIS

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The intelligent data processing technologies are becoming more and more common, because they allow extracting some previously unknown, nontrivial, practically useful and accessible interpretations of knowledge and laws from the raw (unprocessed) data. The research and analysis of nanomaterials structure is one of the most prospective areas of the intelligent data processing usage [1].

There are two tasks of most interest for this area: the clusterization (identifying the data groups or clusters) and the association (search for the patterns between any related events or objects). The application area of clusterization and association include the data segmentation, analyzing the results of scanning probe microscopy, optical research methods (confocal microscopy, optical spectroscopy, etc.) [2]. Thus the implementation of intellectual data analysis methods in manufacturing support systems as well as distributing computing systems (in fact, including the Internet applications) is actual.

In order to perform the data clusterization it is very efficient to use the fuzzy clusterization "c-means" algorithm, which allows not only to form the data clusters, but to determine the probability of a certain piece of data belonging to the current cluster [3].

The search for Association rules is implemented on the basis of the well-known "Apriori" algorithm based on selection of candidates of frequent itemsets of the data. The data retrieval is done through the datasets; after that some association rules are generated basing on the retrieved sets [4].

The algorithm of the developed software tool works the following way. After the receiving the unprocessed data, in case of performing clustering, the following parameters are being input: the number of clusters, the degree of fuzziness of clusters and the minimum level of clustering. After that, the data clusterization is started and the output of the work is a number of the resulting data clusters. In case if performing association, the following parameters are being input: the minimum level of rules support and the minimum level of association rules confidence. The "pretenders" (the most common sets of data) are being allocated and, based on them, the association rules are being created.

Currently an alpha-version of the software tool is developed and being tested. The scalability of a software product can be achieved through the introduction of subsystems in various projects, primarily focused on distributed computing.

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THE EFFECT OF MAIN FILLER DISPERSITY ON THE FUNCTIONAL PROPERTIES OF PHOSPHATE NANOCOMPOSITES

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The application of multi-wall carbon nanotubes (MWCNT) as a functional filler allows provide electro-conductive and shielding properties for phosphate composites [1, 2]. However, it is quite difficult to achieve the uniform distribution of nanotubes in the composite's volume due to the nanotubes tendency to aggregation. This fact requires the introduction of larger functional filler quantity and results in decreasing of strength properties as well as rising in the composite material cost. Previously [2] we reported on the preparation of electro-conductive composites based on alumophosphate binder ($Al(H_2PO_4)_3$) and α-Al_2O_3 as a main filler with particles size ~1 μm and containing 2 mass. % of MWCNT. These materials had the compressive strength properties up to 100 MPa. In order to prepare the composite materials with enhanced characteristics the influence of main filler grain size on functional properties of phosphate nanocomposites has been investigated.

In present research, the composite materials based on alumophosphate binder, main filler composed of AlN and α-Al_2O_3 with different average grain size (1 μm and 150 nm) have been studied. Composite materials were prepared after the hardening of phosphate compositions at room temperature and following thermal treatment at 300 °C. The content of MWCNT in phosphate composite materials varies in the range 0–2 mass. %.

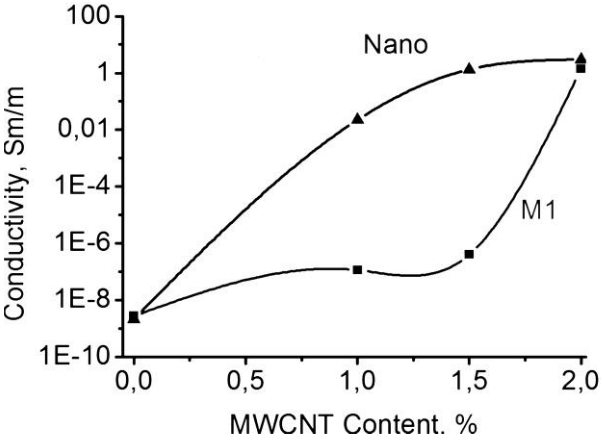

Figure 1. Conductivity of MWCNT-phosphate nanocomposites containing α-Al_2O_3 with particle size 1 μm (M1) and 150 nm (Nano).

The distribution of carbon nanotubes in the composite's volume was studied by scanning electron microscopy (SEM). According to SEM results the more uniform allocation of MWCNT was achieved for the composites containing highly dispersed main filler (particle size 150 nm).

Electro-conductive properties of MWCNT-phosphate composites were studied (**Figure 1**). Obtained results shown that main filler dispersity affect significantly the nanocomposites conductivity. Thus, phosphate composite material containing MWCNT (1 mass. %) and α-Al_2O_3 with particle size 150 nm has the conductivity value of 0.02 Sm / m that is 5 degree higher in comparison with the conductivity of similar one containing α-Al_2O_3 with particle size 1 μm which is characterized with electro-conductive value equal to $1.14 \cdot 10^{-7}$ Sm / m.

The investigation of thermal oxidation stability of phosphate composites with MWCNT in temperature range of 20 – 1000 °C was performed by thermogravimetric analysis (TGA). It was determined that nanotubes oxidation starts at 700 °C that is approximately 200 degrees higher as compare to oxidation temperature of pure MWCNT.

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METAL OXIDE NANOPOWDER SYNTHESIS BY NANOHYDROMETALLURGICAL METHODS

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It was reported that hydrometallurgy had an important opportunity to grow into a new hydrometallurgy, nano-hydrometallurgy, and became an integral component of nanotechnology [1]. In this study several works carried out to synthesis nano powders by using different hydrometallurgy based techniques such as sol–gel, chemical precipitation and solution combustion synthesis.

The effect of boron doping on titanium dioxide powders were investigated by sol–gel method. Starting material was selected as titanium isopropoxide. Change in the structure of boron doped titanium oxide powders was determined by adding different amounts of boron compounds to the sols. Furthermore, effects of synthesis parameters such as agents, molar ratio, aging duration and calcination temperature on anatase to rutile transformation were examined. Thermal analysis and X-ray diffraction techniques were used as well as electron microscopy and chemical analysis techniques for the characterisation and analysis of powders. Anatase particles smaller than 100 nm were obtained by the addition of certain amounts of boron while larger particles of rutile were spherical [2].

A new process of lead recovery directly from spent lead acid battery paste as PbO precursor for making new paste was developed. In this study, the carbon, SO_2 and lead dust emissions were very low towards making new batteries without the use of high temperature pyrometallurgy or the energy-intensive electro-winning processes. By reacting spent lead battery paste with organic reagents and then combusting the organic crystallites, high surface area of PbO was directly synthesised for making pastes for new batteries [3 – 5].

Synthesis of manganese oxide by solution combustion synthesis (SCS) for CO_2 capture was carried out. Urea (CH_4N_2O) and citric acid (C6H8O7.H2O) was used as a fuel material during SCS, while manganese nitrate ($Mn(NO_3)_2$) was used as an oxidant. Surface area of Mn_2O_3 synthesized by using citric acid was calculated as 63.77 m^2 / g when fuel / oxidizer was 1 / 1, at ignition temperature of 250 °C after the calcination at 500 °C. Foam like porous structure of Mn_2O_3 was obtained when citric acid was used as a fuel in SCS. This structure was determined as a candidate for being CO_2 capture material having 27 nm of pore diameter [6].

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WEAK MAGNETIC FIELD STIMULATED PROCESSES OF IMPURITY GETTERING AND ADSORPTION IN SILICON

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It is known that basic properties of semiconductor single crystals which are used in microelectronics and solar power engineering depend on their nanostructure and chemical purity both in the surface layer and in the bulk. As reported in the literature [1, 2], new possibilities of controlling the nanostructure and physical properties of silicon which is a non-magnetic material are provided by the action of magnetic field. In spite of recent progress, there have been a number of unsolved problems, in particular, the problems related to the use of magnetic treatment (MT) as a means of silicon surface activation and, hence, a means of intensification of the processes of impurity gettering and adsorption by the activated surface. On this basis, we set the goal of our study, namely, to determine the role of a weak constant magnetic field (B = 0.17 T) as a factor that may facilitate both gettering and adsorption of impurity centers, including recombination centers in silicon.

By means of atomic force and magnetic force microscopy as well as secondary ion mass spectrometry we have established that treatment of silicon crystals in weak magnetic fields creates impurity enriched surface nanostructures. At the surface and in surface layers of silicon MT increases C, Na, K, Ca, Al and other impurity concentration 3 – 5 times. Thus the impurities that diffused from the bulk to the surface not only change the topology of the surface, but also transfer it into a magnetic field activated state.

Additional studies involving X-ray spectroscopy have shown a threefold increase in oxygen paramagnetic impurity concentration in the surface layers and at the surface of silicon crystals exposed to MT. The latter may indicate that intensified is not only the process of gettering, but also that of adsorption, which may lead to silicon dioxide (SiO_2) film thickness growth.

Indeed, by means of ellipsometry we have found that oxide nanostructured objects with clearly expressed stepped structure are formed at the magnetic field activated Si surface at the expense of oxygen adsorbed from the ambient. So, the magnetic field induced changes in the surface morphology and in the character of cross-sections relief may be a result of impurity gettering by the silicon surface and a result of changes in surface sorption properties.

Magnetic treatment of Si crystals may be an economical way of controlling the structure and impurity state as well as the surface morphology of silicon crystals and, hence, the physical properties of silicon which is the basic material for microelectronics and solar power engineering.

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INJECTABLE BIOPOLYMER–HYDROXYAPATITE HYDROGELS

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Hydrogels are soft and wet materials, composed of a three-dimensional polymer network in which a large amount of water molecules are interposed. Some recent studies have indicated that hydrogels, especially those derived from natural proteins and polysaccharides, are ideal scaffolds for tissue engineering, since they not only offer several advantages over synthetic polymers and inorganic scaffolds but also provide a three-dimensional (3D) environment and morphology close to the extracellular matrix of native tissues. In this work the hydrogels based on hydroxyapatite (HA) and Chitosan (CS) with addition of sodium alginate (Alg) were synthesized by *in situ* precipitation method. Structure, morphology, chemical and phase composition of the HA / CS and HA / CS / Alg hydrogels were characterized by TEM, FTIR and XRD. Hydrogels consist of low crystallinity calcium deficient hydroxyapatite (JCPDS 9 432), the needle-like crystallites with an average size 25 nm. The introduction of Alginate powder into HA / CS hydrogel solution demonstrate the viscosity enhancing of the HA / CS hydrogel due to polyelectrolyte reaction between Alginate and Chitosan macromolecules. Two natural polymers and partially released from hydroxyapatite Ca^{2+} ions formed a matrix by crosslinking the polymer macromolecules through hydroxyl, amino and carbonyl groups. These processes promote the formation of a more stable structure of HA / CS / Alg hydrogel as compared to HA / CS. The structural integrity and degradation tests have demonstrated that HA / CS / Alg1.0 saved its initial shape after 7 days of shaking in SBF solution, meanwhile for HA / CS, a structural decay was observed. The HA/CS hydrogel had completely lost its volume support after 1 day shaking in SBF. Thus, the ability of HA / CS hydrogel to maintain its shape with implantation into bone tissue defect may be enhanced with alginate addition, but alginate content more than 1 w/w % reduces the hydrogel plasticity, increases the swelling and accelerates the shape decay.

ESTIMATION OF KINETICS PARAMETERS OF DEHYDRATION AND CRYSTALLIZATION PROCESS OF ZrO_2 – 3 mol. % Y_2O_3 XEROGELS SYSTEM MODIFIED UNDER CONDITIONS OF HIGH HYDROSTATIC PRESSURE

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Pressure and temperature is an important tool for the synthesis of almost all technologies and forming oxide powders. In the case of zirconia based systems which have more polymorphic forms in depending on the P-T conditions, the pressure can be used as the control factor of material properties.It is known that the characteristics of crystalline zirconia nanoparticles (particle size, specific surface area, etc.) greatly depend on the xerogel structure of zirconia nanoparticles. Xerogel zirconia is a skeleton of interconnected amorphous nanoparticles of zirconia with hydration shell and supplementing its porous space. Oxide nanopowder formation occurs in a series of sequential dehydration reactions, crystallization, destruction, adherence, under heat treatment conditions of xerogels. As shown earlier the xerogel modification under HHP conditions results to nonmonotonic change of state of hydration components and structural organization of amorphous xerogel [1].The main goal of this paper is the estimation of kinetic parameters (activation energy, Avrahami"s parameter and reaction equation), dehydration and crystallization processes of xerogels modified under the HHP (100 – 1000 MPa) by DSC. The kinetic parameters had estimated by the method of Kissinger [2] and Avrami–Dzheziorni [3].

It has been shown that the estimated activation energy of the dehydration process nonmonotonically changing in depending on the amount HHP with an extremum at 600 MPa. Whereas, the dependence of the activation energy of the dehydration process on the degree of connectivity of the aqueous component with the xerogel surface nanoparticles is monotonic.Based on analysis of the estimated water densities occurring in the experiment thermodynamic conditions, and the $P - T$ - diagram of the water state found that the probability of reorganization in the structure of the hydration shell of xerogel is connected with water's phase transitions [4].It has been found that the kinetic parameters crystallization is monotonic in depending of theHHPvalue.This is demonstrated in a monotonic increasing of the activation energy process and the changing of the crystallization mechanism from volume growth of crystallizing particles at the constant rate of nucleation to volume growth with increasing nucleation.

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GEOMETRY INDUCED DOPING IN THIN SILICON NANO-GRAITING LAYER

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Main goal of our research is to fabricate and characterize nanostructured thin layers for studying it's electronic and thermoelectric property. Fast development of nanotechnology gives possibility to realize few nanometre pitch size of structures [1, 2]. Theoretical study [3, 4] and simulation [5] shows that electronic, thermoelectric and electron emission property changes apparently, when grating pitch size is comparable to electron's de Broglie wavelength. Nano-grating imposes additional boundary condition to electron wave function and some quantum states forbid, electrons from prohibited quantum states have to move up and occupy available state with higher energy. Some electrons have to jump from valence band to conduction band, because quantum states in valence band are prohibited and all upper states are occupied. So electron concentration in conduction band increases and we will get geometry induced doping or G-doping. G-doping is similar to donor doping, but it does not require ionized impurities. That's allows high carrier mobility and temperature independent carrier concentration.

Nano-grating areas were fabricated using laser interference lithography with high coherent 375 nm laser beam. Nano-structured square islands (0.3×0.3 mm^2) were shaped on thin device layer of silicon on insulator (SOI) wafer. SOI wafer was chosen because this material is widely available. Reactive ion etching was used to etch down structured areas. Four Ohmic contact field were formed using Ti / Ag material which was deposited on top of Si. $I - V$ characteristics of nanostructured arias using 4W and 2W methods shows 2 – 3 order magnitude reduction of resistivity at room temperature (300 K). Resistivity of Si plane layer was 10 Ohm cm and after structuring it become $5 \cdot 10^{-2} - 8 \cdot 10^{-3}$ Ohm $\cdot$ cm. This reduction is in agreement with G-doping theory. Value 10^{-2} Ohm $\cdot$ cm corresponds to "impurity" concentration of $3 \cdot 10^{18}$ cm^{-3} (phosphorous in Si). We also studied resistivity anisotropy with temperature range 0.2 – 1 to 300 K. Nano-grating fabrication does not require ultra-high technology and it can be used for solar cells, photovoltaic devices also for high frequency electronic and power electronics.

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SYNTHESIS OF NANOSTRUCTURED ZnO DOPED SiO_2 THIN FILMS BY SOL–GEL DIP COATING TECHNIQUE

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ZnO is one of the most widely used semiconductors for many different applications such as solar cells, gas sensors, and photocatalytics [1]. On the other hand silica based nanostructuredmaterialsare prominent candidates for microeletronic, optical and optoelectronical applications [2]. Nanostructured ZnO–SiO_2 thin films have been found to present many interesting photoluminescence properties, such as great enhancement of UV emission, white-light emission, and adjustable visible emission [3]. Therefore they found usage in very different applications such as, photonic crystals, photocatalysts, gas sensors, vacuum fluorescent display and varistors [4, 5]. Nanostructured ZnO–SiO_2 films have been prepared using various techniques such as sputtering, chemical vapor deposition, chemical etching and sol gel process [4]. Among them, the sol-gel is considered to be one of the most efficient techniques for the synthesis of nanostructured silica based thin films and represent a simple and low-cost processing alternative to the vacuum deposition techniques [5].

In this study nanostructured ZnO doped SiO_2 thin films were deposited on glass and silicon substrates by sol-gel dip coating technique. The effect of ZnO nanopowder addition into the starting SiO_2 sol and different dipping-rising cycles on the properties of the films were investigated. Microstructural properties of the films were characterized by cross-sectional SEM observations and EDS was used to determine the film composition. Spectrophotometer has been used to measure the optical properties of the films. The results demonstrated that homogenous and well-adherent nanostructured ZnO doped SiO_2 thin films with very high transmittance properties were successfully deposited.

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HYBRID ORGANIC / GaN NANOWIRE STRUCTURES FOR SOLAR CELL APPLICATIONS

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Direct harvesting of solar energy is no doubt an important part of future energy technology. Rapidly growing solar energy market generates huge demand on novel solutions aimed at both increasing the effectiveness of photovoltaic devices and keeping the per kilowatt price of solar installations within realistic boundaries. Newly emerged class of polymer solar cells has recently demonstrated rapid increase in effectiveness at the same time remaining relatively cheap and, more importantly, scalable technology.

In this work we present our results on fabrication and characterization of hybrid solar cell combining π-conjugated polymer with GaN nanowires grown on conductive substrate. Superior electrical properties of nanowires serve the purpose to enhance conductivity of light-absorbing layer, which in case of organic photovoltaics is limited by low charge carrier mobility.

Structures of poly(3-hexylthiophene-2,5-diyl) (P3HT) [1] and GaN nanowires were fabricated and characterized for this study. Self-assembled GaN nanowires were grown using Plasma-Assisted Molecular Beam Epitaxy technique. Bottom contact to GaN nanowires was provided through nucleation layer which is an amorphous material of metallic electrical conductivity deposited on silicon substrate. P3HT solution was put on the array of nanowires by spin-coating resulting in a layer of p-type polymer with embedded n-type nanowires. The active layer was covered by PEDOT:PSS electron blocking coating. Top contacts to a solar device are made using transparent indium tin oxide (ITO) layer or by depositing thin metal pattern on the surface of the device.

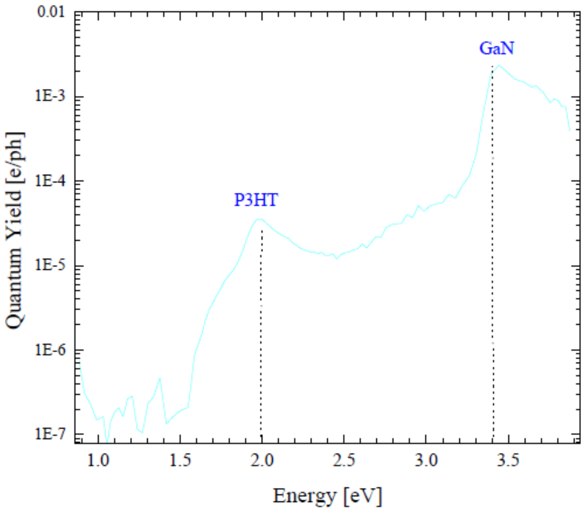

Figure 1. Photocurrent spectrum.

Morphology studies show that the space orientation of nanowires remains close to perpendicular to the substrate surface independently from nucleation layer thickness, result consistent with reported for growth of self-assembled nanowires on different amorphous substrates [2]. Quantum yield spectroscopy measurements were made in closed circuit mode. The results (see **Figure 1**) show that structure exhibits photogenerated current maxima at 1.9 and 3.4 eV energy light which correspond to bandgap edge of P3HT and GaN respectively. This means that light generates electron-hole pairs in both materials and that there is efficient transfer between the materials. The observed direction of photocurrent confirms that GaN works as n-type layer and P3HT is a p-type layer in this heterostructure.

Electrical characteristics of nucleation layer-GaN interface were measured showing good ohmic contact between the components. Dependence of structure charge carrying properties on GaN doping is shown as well as electrical characteristics of polymer–GaN interface.

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THE S-DOPING OF TiO_2 NANOPARTICLES FOR ENHANCED EFFECTIVITY OF PROTON CONDUCTING MEMBRANES

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Current proton conducting membranes fuel cells for various applications, which employ perfluorosulfonic polymer nafion membranes, yield the best performance around 80. The operation of fuel cells at this temperature has a number of shortcomings which can be avoided by raising the temperature to 120 °C and even higher. However, nafion membranes experience a rapid drop in conductivity as temperature increases to above 100 °C, and not suitable in high-temperature operation. In this context, the improvement of the existing membranes is pursued, namely composite membranes consisting from nafion, and inorganic nanoparticles are considered.

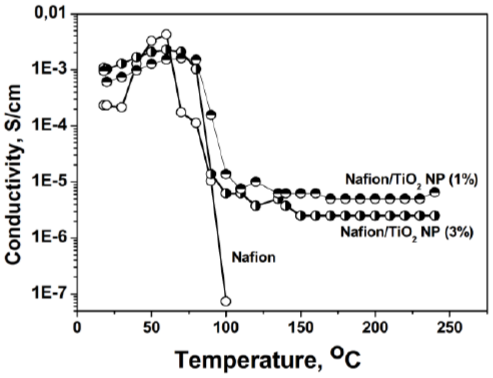

Figure 1.

In this study, we specifically focus on the effect of additivity of doped TiO_2 nanoparticles on the performance of the nafion / TiO_2 composite membranes in high temperature. In the framework of the research on the nature and mechanism of action by XPS, SEM, XRD, TPD MS, optical and vibrational spectroscopy investigated the properties of active titanium-oxide additive polymer membranes. Established, that modified titanium oxide nanoparticles due to the nature of their composition and structure have a strong capacity for coordination of water molecules on the surface, causing the formation of hydrated grid structures in composite labile protons and maintenance of structures percolation cluster hydrophilic channels in membranes. It found that the conductivity of the nafion / TiO_2 composite confirms the formation of a percolation cluster, in consequence, with mesoscopic ordering and polarization of water molecules on the strong acid groups of doped titanium dioxide species to form hydrated Eigen-to-Zundel-type ions in a frame of Grotthuss conductivity mechanism. Preliminary tests of proton conductivity (the direct injection of protons) that was carry out on the composite membrane, has highlighted the benefit of doped titania nanocomposites introduction on the conductivity in the temperature range up to 240 °C, that maintained at (10^{-5} – 10^{-3} S), compared to the commercial nafion membrane (**Figure 1**). The above may be a prerequisite for effective behavior composite polymer membrane in conditions close to the operating conditions of fuel cells.

NEW DEVELOPMENTS ON HIGH EFFICIENT SOLER CELLS

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Since the last conference Nano – 2014, the technology of high efficient solar cells and solarmodules have been improved. In addition to the following technologies:

- Crystalline silicon modules with efficiencies now of more than 22 %:
  - Bifacial solar cells (requiring quite a distance behind the modules),
  - Selective emitter solar cells,
  - n-type solar cells with heterojunctions.
- Concentrator modules based on III–V-multijunction cells, with efficiencies now of more than 40 % [1],

The EU-Project “Full Spectra”, with an intermediate (impurity) band in the forbidden zone led to an extended spectral range of sensibility, based on early investigations (see [2]).The Intermediate Band (IB) solar cell is a new concept to increase simultaneously the current of a solar cell without reducing substantially the voltage [3]. This leads to an efficiency increase.

The efficiency limit for an ideal IB solar cell is about 63 % vs.40 % for an ordinary solar cell under the same hypotheses. There are now over 60 research centers worldwide working on the IB solar cells.

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TRIBOCHEMISTRY VERSUS NANO-TRIBOLOGY

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The paper should discuss a connection between the aspects of modern *nano-tribology* [1] and the research of the seventies and eighties in the field of *tribochemistry* [2]. *Nano-tribology* is the science of friction, lubrication and wear, considered and measured in the picometer to nanometer scale. In such a scale are proceeding the elementary processes of mechanical interaction of moving (in the nanoscale *impacting*) solid surfaces one to another (called friction). *Tribochemistry* is the science of the chemical conversions taking place under frictional mechanial treatment. Excellent experimentators have described such interesting tribological Effects as "Non Wear Friction" [3] or "Magma-Plasma-Model" [4]. However, the "revolutionary" results as really *non wear* in the tribological system copper / bronze / glycerol [3] and the oxidation of copper with carbon dioxide (with *negative* affinity) [4] or the "tribogalvanic" deposition of zinc *against* the electrochemical series [5], albeit experimentally observed and documented, have not be shown by means of nanoanalytical devices until now. Unless they *are* in fact nanotribological proeesses in atomic dimensions. The *time line* of tribochemical interaction between solids after one mechanical impact is supposed by following states [6]: *triboplasma* (stochastic procesesses); *edge- and post-plasma* (relaxation of triboplsma, recombination of plasma products (coupled, non revesible thermodynamic processes) and at least approaching to the thermostatical (thermodynamical) eqilibrium (mechanically activated reactions (non reversible thermodynamic procesesses described by thermostatics).

As an example I want to deduce the possibility of *direct watching* of the processes in a fictive or non fictive "triboplasma" by means of a modified nanotribometer. Nanotribometers [7 – 9] are special scanning probe microcopes (SPM), using special cantilever constructions for multi-purpose friction measuring in the nano scale. The task will be to watch *directly* (live) the above mentioned triboplasma processes by means of a modified SPM: A *Tandem SPM* with the possibility of *simultaneous* observation of the action of an AFM by means of a *coupled* STM. This should be realised by a double tip (tandem) cantilever, one of the tips (electrically isolated) is in direct mechanical interaction with a metallic surface (AFM), the second, electrically conductive, without direct touching of the sample, serves as STM. *"Big Brother is Watching You"* (George Orwell).

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TANDEM NANOSCOPE

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I would like to enclose a poster presentation for discussion over the possible design of a novel "Tandem Nanoscope".

MODELING OF THE PHASE DIAGRAM AND KINETICS OF MATERIALS FRAGMENTATION MODES UNDER SEVERE PLASTIC DEFORMATION

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At present, metals are subjected to the different processing forms for the achievement of the high physical and mechanical properties (the high strength, hardness, crack resistance, elasticity, plasticity, viscosity, wear resistance, etc.) The application of the methods of severe plastic deformation (SPD) allows to obtain the bulk metallic samples with almost pore-free submicrocrystal (SMC) or nanocrystal (NC) structure, which cannot be obtained by ordinary thermomechanical processing. The application of repeated plastic deformation of shear at the expense of heavy-loaded application in rather low temperatures conditions is the base of SPD methods. It leads to the formation of structure with grain sizes about 100 nm and downward [1], which is rather important for modern nanotechnological process.

Recently, the construction of the theoretical models allowing to describe the processes of microstructure grinding of metal at SPD acquires significant importance. As a result, the special approach within nonequilibrium evolutional thermodynamics is developed [2 – 4]. It helps to establish the course of nonequilibrium processes (heating and defect generation) and transformation nature of internal energy during material processing. Consideration of bounded multidimensional polynomial relationship for density of internal energy, allows us unambiguously reflect the nature of grains fragmentation and attendant processes of formation of limiting structure under the SPD. Therefore, the grain boundary and dislocation are considered as the most important types of structural defects.

The phase diagram of fragmentation modes in approximation of a two-defect model is obtained. It sets the conditions of formation of various types of limiting structures under the SPD. Besides, the formation conditions for two limiting structures are found. They correspond to the mode, in which there is a mixture of different grain sizes. The evolution of nonequilibrium variables at SPD is investigated in details.Two basic cases of initial conditions are considered for calculation. Its correspond to the nonhardened metals or alloys and to the defectsfull materials, which have the high strengthening properties. It is shown that various types of stationary structures are formed depending on the values of shear strain and the initial states of the material. The defects density of these steady-states corresponds to experimentally observed regularities (with the linear size of grains 100 nm and dislocations density within range of 10^{15} – 10^{16} m^{-2}). Moreover, the close interaction of the defects of different structure levels in the course of steady-states establishment is observed. It is revealed that nonequilibrium variables undergo structural and phase transition. As the result, the evolution of defects density performs sharp transition. It is established that formation of limiting structures is followed by both processes of dislocations accumulation and grains grinding on the one hand and annihilation of dislocations and grains growth on the other.

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A STUDY ON THE EFFECTS OF FUNCTIONAL ADDITIVES ON THE SELF-PROPAGATING HIGH-TEMPERATURE SYNTHESIS OF NANO SCALE TiB_2

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TiB_2 has unique properties such as high hardness, strength, melting point, thermal and electrical conductivity, etc. It is a transition metal boride and it has hexagonal crystal structure with space group of P6/mmm. The melting point of TiB_2 is about 3225 °C [1 – 4]. Its covalently bonded atomic structure provides the hardness values as high as 45 GPa [5]. Self-propagating high-temperature synthesis (SHS) is employed to synthesize advanced ceramic powders in nano scale (TiB_2, B_4C, Si_3N_4, etc.). SHS reactions are highly exothermic. So, the propagation of reactions and the yield of reaction products continue in self-sustaining mode without any additional heat or energy [6].

In this study, TiO_2 and B_2O_3 powders were mixed with various stoichiometrically required amounts of Mg powders as reductant. SHS experiments were conducted under air and argon atmospheres respectively. The effects of functional additives (NaCl and $MgSO_4 \cdot 7H_2O$) were investigated with the different addition ratios. SHS products were leached in HCl media to purify their TiB_2 contents. The optimum SHS parameters were determined as stoichiometrically 100 % Mg addition and Ar process atmosphere. Mg content of the experiment which was conducted with the optimum parameters was measured as 0.81%. Besides, its specific surface area was measured as 6.42 m^2 / g and its average grain size was about 200 nm. Addition of NaCl and $MgSO_4 \cdot 7H_2O$ increased the amounts of impurities (e.g. TiO_2, Mg based oxides) in the synthesized powders and in the leached TiB_2 powders. But, specific surface area values of the leached powders were remarkably increased with the addition of NaCl. Measured values were 11.50 m^2 / g for 2.5 % NaCl addition ratio and 11.78 m^2 / g for 5.0 % NaCl addition ratio. On the contrary, $MgSO_4 \cdot 7H_2O$ addition dropped the specific surface area values.

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OBTAINING OF ALUMINUM-MATRIX COMPOSITES MODIFIED WITH BORON NITRIDE

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The development of the alloys based on aluminum with fine-grained structure which are characterized by the high level of physical, mechanical and operational properties is an actual task today. Generally impurity modifying, accelerated hardening and inverting of microstructure of billets are used for these purposes allowing to increase mechanical and operational properties of castings not only from primary but also from low-cost secondary alloys [1]. Additives of micro- and nanostructural refractory particles as impurity modifiers (fillers) enable to change effectively the structure of aluminum alloys. They contribute to its fine crushing and increasing of the mechanical and tribotechnical characteristics of aluminum matrix composite materials (CM) [2]. Carbon nanomaterials (carbon nanotubes, fullerenes, detonation synthesis ultradispersed diamonds, shungite carbon) are of widespread application for these purposes [3].

Different ways are offered to improve the interaction of the refractory micro- and nanoparticles with aluminum melt and to increase the uniformity of their distribution in a matrix. So, an effective approach has been developed in the works [4] relating to the production of the reinforcing nanostructured composite refractory ceramic fillers based on hexagonal boron nitride and silicon oxide. Their use enables to disperse effectively the structural components of silumin and leads to the essential increase in physical, mechanical and tribotechnical characteristics of the composites. At the same time a high pressure during sintering of such composites will contribute to the structure stabilization and phase structure of both the filler and the matrix that is currently important when obtaining nanostructural composite materials [5].

The purpose of this work was the investigation of the influence of additives based on the refractory particles of nanostructured cubic boron nitride on the structure and microhardness of the aluminum-matrix composites obtained under high pressure.

It has been shown that the introduction of additives of nanosructured BN with aluminum coating in aluminum matrix inhibits growth of the aluminum grains in the high temperature treatment region and increases microhardness of the composite materials. The technological schemes of high pressure treatment of aluminum-matrix composites such as Al–BN have been developed.

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ELECTRODES BASED ON Ti DIOXIDE, MODIFIED BY Ag AND Au NANOPARTICLES FOR ELECTROCHEMICAL SENSOR OF OXYGEN

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Electrodes for electrochemical sensor of oxygen dissolved in biological liquids have been developed, the operation of which is based on the oxygen electroreduction process. The cathode materials were TiO_2 based films doped with Ag or Au nanoparticles prepared via photo- or thermoreduction of metal ions introduced into bulk or adsorbed on the film surface [1]. Noble metal doping effect on the photoelectrochemical properties and electrocatalytic activity in the reaction of oxygen electroreduction were investigated. TiO_2 and TiO_2 / ZnO films with the Ag or Au nanoparticles distributed in the matrix and on the surface were characterized by TEM, AFM, XRD and UV-Vis spectroscopy. Band gap energy and the position of flat band potentials of TiO_2 / M and TiO_2 / ZnO / M heterojunctions were estimated by photoelectrochemical measurements [2] which showed the cathodic shift of the flat-band potential position in comparison with unmodified TiO_2 electrodes.

The oxygen electroreduction process was investigated in physiological (0.9 %) and isotonic (7.5 %) solutions of NaCl. It has been found, that oxygen reduction polarisation curves exhibit one polarographic current wave at potentials of – 0.40 to – 0.9 V (against silver–chloride reference electrode). The mechanism of oxygen reduction on the electrodes under investigation is determined by mixed kinetics. We have shown that the limiting oxygen reduction current for the semiconductor electrodes is diffusion current, the dependence of limiting current on dissolved oxygen concentration being linear.

It is shown that TiO_2 modification with Ag and Au nanoparticles improves catalytic activity in the reaction of oxygen electroreduction: lead to the decrease of overvoltage in the process of oxygen electroreduction and extend the potential range for the concentrations of soluted oxygen determination. The greatest sensitivity to dissolved oxygen has been reached for the electrodes TiO_2 – 1 % ZnO–Ag and made $(1 - 2) \cdot 10^{-5}$ g / l. The correlation between electrocatalytic activity of electrodes and energy position of conduction band E_{fb} is determined.

It is shown that electrodes based on TiO_2 and TiO_2 / ZnO modified by Ag or Au nanoparticles have high stability and reproducibility of characteristics in the process of O_2 electroreduction in physiological and isotonic solutions of NaCl and are perspective for use in electrochemical sensor of the dissolved oxygen.

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TAILOR-MADE PLASMONIC NANOPARTICLES FOR SURFACE-ENHANCED RAMAN SPECTROSCOPY AND IMAGING

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Surface-enhanced Raman scattering (SERS) has become a mature vibrational spectroscopic technique during the last decades and the number of applications in the chemical, material, and in particular life sciences is rapidly increasing [1]. In addition to normal Raman spectroscopy, SERS requires plasmonically active materials, for instance noble metal colloids, which support localized surface plasmon resonances.

This lecture gives an overview on the rational design and synthesis of functionalized noble metal colloids for chemical and bioanalytical applications of SERS. After a brief introduction on the theoretical foundations of SERS, two different topics from the chemical sciences with results from our group will be covered. In both cases plasmonic nanostructures with tailor-made physical and chemical properties play a key role.

Immuno-SERS microscopy (iSERS) for tissue-based cancer diagnostics employs target-specific colloidal SERS probes in combination with Raman micro-spectroscopy. SERS-labeled antibodies allow the selective and sensitive localization of the corresponding antigen in tissue specimens. The properties of the colloidal SERS probes [2] (**Figure 1**) are crucial for the success of iSERS experiments. Signal brightness, stability and robustness as well as steric accessibility for bioconjugation are few very important aspects. For instance, small Raman reporter-functionalized clusters of noble metal nanoparticles (NPs) are very bright SERS labels due to plasmonic coupling. Small clusters of AuNPs were further used for iSERS imaging on prostate biopsies. Current work in our laboratories and future developments of this innovative iSERS imaging approach will be discussed.

The second part of the lecture covers label-free monitoring of chemical reactions catalyzed by Pt, Au and Ag nanoparticles. Bifunctional nanoparticles exhibiting both high plasmonic and catalytic activity are required, but not routinely available. We designed and synthesized Au/Pt nanoraspberries as well as Au/Au and Ag/Ag core/satellite superstructures for this purpose (**Figure 2**) [3 – 5]. Electron microscopy demonstrates the high uniformity of the particles. Computer simulations predict very high plasmonic activity due to plasmonic coupling, resulting in several hot spots. For proof-of-concept studies 4-nitrothiophenol, which is present as a self-assembled monolayer on Au and Ag surfaces, was chosen. The reduction to 4-aminothiophenol can be achieved either by chemical hydride agents or by a combination of hot electrons and protons. Current work from our group on temperature-controlled microfluidics for kinetic reaction monitoring as well as future directions for the use of hot electrons for driving chemical reactions will be discussed.

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Si / SiO_2 POROUS TEMPLATE FOR Cu NANOSTRUCTURES SYNTHESIS

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In this work, n-Si / SiO_2 (Cu) structures with different morphologies of copper deposits are produced using the template synthesis method [1]. Deposition of Cu nanostructures and their structural features are thoroughly studied, and mechanisms for formation of compact and dendrite-like deposits in the pores of the SiO_2 template on the n-type single-crystal silicon substrate are established [2]. Spatially separated copper dendrites are obtained and used to investigate the efficiency of Raman scattering enhancement using the aqueous solution of the rhodamine 6G dye (**Figure 1**). Factors affecting oxidation of copper nanostructures are discussed, and methods for protecting Cu dendrite surfaces against corrosion and increasing the signal enhancement factor are discussed.

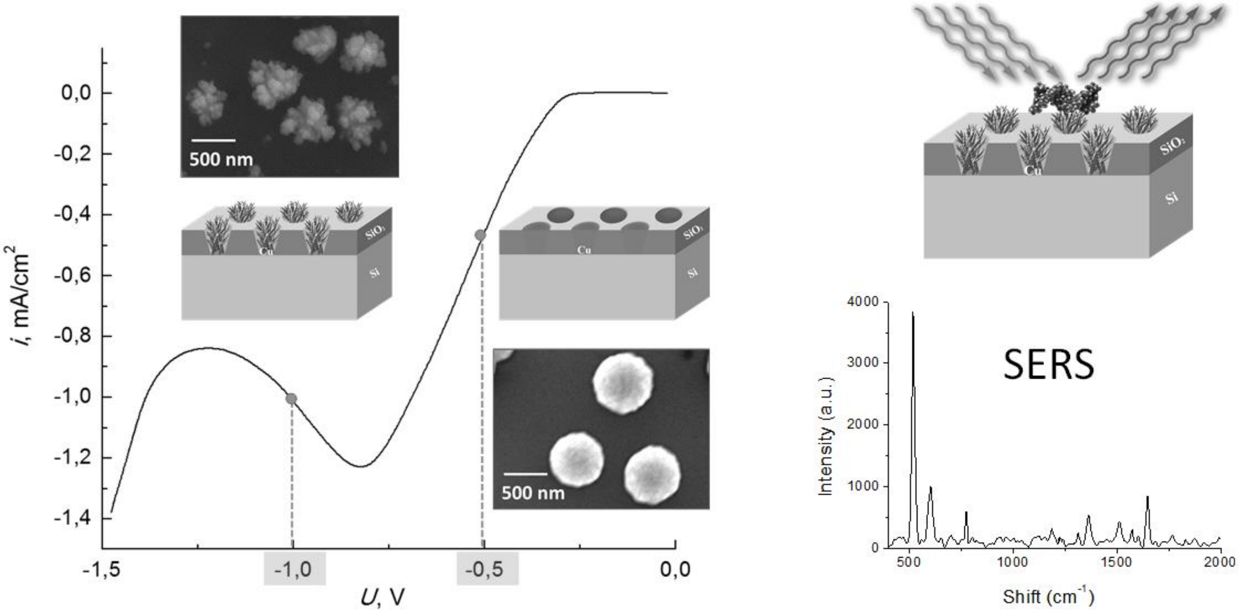

Figure 1. Potentiodynamic current–potential cathode curve of Cu deposition on the n-Si substrate with SEM images and SERS spectrum of the 10^{-6} M rhodamine 6G aqueous solution.

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MAGNETIC AND DIELECTRIC ANISOTROPY OF BaM / NANOCARBON / POLYMER COMPOSITES WITH ALIGNED FILLER

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Recently, carbon based polymer composites have gained significant popularity because of their low cost, facile synthesis and ease of processing. Their properties can be improved due to presence of barium hexaferrite (BaM), with a basic composition of $BaFe_{12}O_{19}$, which is one of the most commonly used material in hard-magnetic, magnetic recording, magneto-optics, magneto-electrics, magnetic gels [1] and high-frequency applications [2]. The presence of BaM nanoparticles in the composite enhances the space charge polarization, natural resonance, multiple scattering and the effective anisotropy energy leading to a high electromagnetic interference shielding effectiveness [3].

Graphite nanoplatelets (GNPs) / BaM / polymer and multiwall carbon nanotubes (MWCNTs) / BaM /polymer composites with uniform and aligned by magnetic field BaM distribution were prepared. The content of MWCNTs (GNPs) in composites was 2 – 5 wt. %, the content of BaM was 27 wt. %.

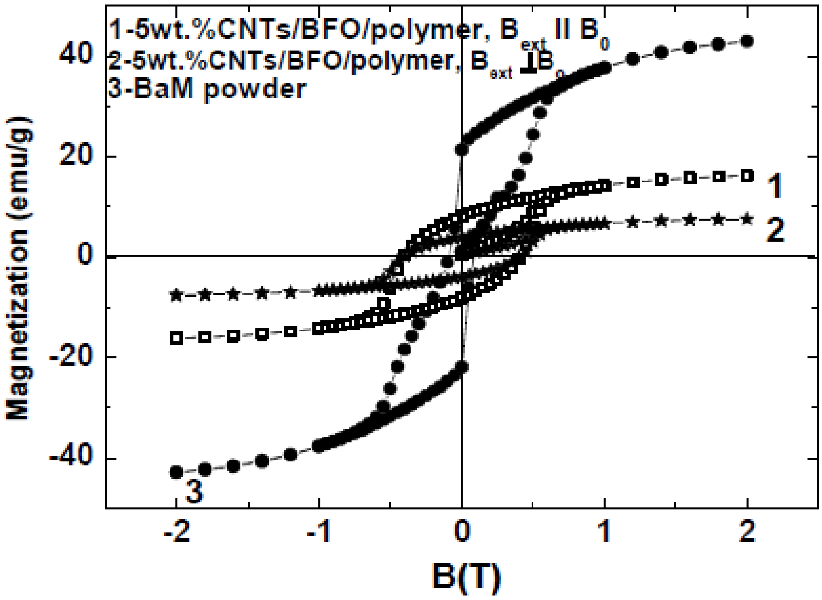

Figure 1. Field dependence of magnetization of nanocarbon / BaM /polymer composites.

The results of the field dependence of magnetization (**Figure 1**) and the frequency dependence of dielectric permittivity of the investigated composites are presented. At the composite formation the saturation magnetization decreases and greatly increases the coercive force as compared with the BaM powder itself. Furthermore, different measurement geometry has revealed anisotropic field dependence of magnetization and frequency dependence of permittivity for the aligned composites. At the parallel orientation of external field B_{ext} to the direction of magnetic field B_0 at the composites synthesis the samples have a greater magnetization than at the perpendicular orientation. Besides, the impact of the carbon filler type on the effectiveness of BaM alignment under the influence of magnetic field and the nanocomposites magnetic and dielectric properties is considered.

The results suggested that the as-prepared aligned BaM / nanocarbon / polymer composites showed great potential as a promising material for permanent magnets and a new type of microwave absorbing shields formation.

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GOLD NANOPARTICLE PLASMON RESONANCE IN LAYERED Au NPs / DIELECTRIC SPACER / Al FILM NANOSTRUCTURE: EFFECTS OF SPACER THICKNESS

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A particularly interesting plasmonic system that recently is under study is that of a metal NPs interacting with a metal film. This system has been predicted to display a lot of interesting optical phenomena caused by the coupling of the NPs with the film through the field of surface plasmons excited in the NPs, e.g. Refs. [1, 2]. The study of optical spectra (absorption, scattering) of the metal NPs separated controllably from a metal film using the dielectric spacer gives the possibility to probe the dependence of coupling effects on the distance between the NPs and film.

The studied plasmonic nanosystem is following. The dense 2D monolayer of Au NPs was fabricated on glass substrate. Then the Au NPs' layer was covered by dielectric film of shellac. The thickness of shellac film was different in different parts of the sample varying in the range of 3 – 36 nm for sample S1 and 30 – 200 nm for sample S2. Above the shellac film, the aluminum film of 50 nm thickness was deposited. AFM gave the following Au NPs' layer parameters: NP size $d = (22 \pm 8)$ nm; mean interparticle distance $D = (40 \pm 10)$ nm. Thus, the studied Au NPs' layer is quite dense.

The absorption spectra of above mentioned three-layer nanostructure were measured at room temperature. We have obtained that coupling of surface plasmon resonance (SPR) in Au NPs with Al film leads to substantial enhancement (5. 3 times) of the SPR magnitude and its appreciable red shift if comparing to the case of Au NPs without Al film. The increase of SPR magnitude at the decrease of spacer thickness from 200 to 70 nm is probably due to the following processes. First one is the excitation of propagating SP polaritons in the Al film through the near field of localized SPs in Au NPs. Second one is the redirection of the external incoming light as well as the light scattered by NP by Al film back to layer of Au NPs with the subsequent absorption of the light by Au NPs. At thickness values lower than about 70 nm the decrease of dipolar SPR magnitude and the concomitant appearing of the quadrupolar SPR occur at the decrease of spacer thickness. This behavior is due to the hybridization of the dipolar and quadrupolar plasmons in the Au NP caused by the symmetry-breaking introduced by the presence of the Al film. As a result, the quadrupolar resonance acquires part of the "bright" character of the dipolar mode becoming easily visible on the absorption spectrum. Correspondingly, the dipolar resonance becomes darker, i.e. its magnitude decreases. The origin of observed appreciable (160 nm) red shift of SPR in Au NPs at the decrease of Al film thickness from 200 to 3 nm is the coupling of Au NPs and Al film through the plasmonic field. The decrease of spacing between Au NPs layer and Al film makes the coupling stronger that results in the red shift of SPR.

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TITANIUM MANGANESE OXIDE SYNTHESIS BY SOL–GEL COMBUSTION ROUTE

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Solution combustion synthesis (SCS) is a versatile, simple and rapid process, which allows effective synthesis of a variety of nanosize materials. Despite of the conventional processes, this process involves a self-sustained reaction in homogeneous solution of different oxidizers (e.g., metal nitrates) and fuels (e.g., urea, glycine, hydrazides). This process not only yields nanosize oxide materials but also allows uniform (homogeneous) doping of trace amounts of rare-earth impurity ions in a single step [1, 2].

TiO_2 has a wide usage area in nanoscience applications such as solar cells, medical applications, pigments in dye. It has large band gap (3 eV for rutile and 3.2 eV for anatase) so to improve the photoactivity, the change of the equilibrium concentration of electrons or holes and the light absorption TiO_2 is doped by different admixtures which are transition metals, nitrogen, sulphur, and other. Synthesis procedure and dopant metal are important in order to final product's physical and chemical properties. Manganese oxide is a good alternative for dopant material. TiO_2 / MnO_x seems to present interesting optical and photocatalytic properties, as well as it may be a perspective material for solar energy conversion [3]. Chemical looping is a process in which a solid, usually a metal, carries oxygen from air or steam to a fuel gas and converts it, avoiding a direct contact between the both reactants. This oxygen carrier is usually bound with an inert material that does not participate to the reactions [4]. Chemical looping oxygen uncoupling is a particular case of chemical looping that enables gas-solid reactions like oxygen with a solid fuel instead of solid-solid ones like metal oxides with coal or biomass. Manganese oxides are one of the materials to be used for the oxygen carrier systems [5].

In this study, titanium manganese oxide nanoparticles were synthesised by sol–gel combustion method. Urea (CH_4N_2O) and citric acid ($C_6H_8O_7 \cdot H_2O$) was used as a fuel material during solution combustion synthesis, while manganese nitrate ($Mn(NO_3)^2$) and titanium chloride ($TiCl_3$) were used as an oxidant. The structure, morphology and chemical composition of the samples were characterized by using wet analysis as well as XRD, SEM, and EDS methods. Surface area of synthesised particles was determined by BET analysis.

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SYNTHESIS AND CHARACTERIZATION OF THIN FILMS FOR WEAR-RESISTANCE, MECHANICAL, OPTICAL AND OPTOELECTRONICAL APPLICATIONS: A REVIEW

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In this review, we summarize thin film deposition and characterization studies realized in our "MacrotoNano" research team in Istanbul Technical University since 15 years. Examples include B_4C, BCN, WC, WCN and SiC. The depositions were made by reactive / DC magnetron sputtering. Sophisticated characterization techniques were used to elucidate the properties of the deposited films. Elemental composition of the films was measured by electron probe microanalysis (EPMA). Field-emission gun scanning electron microscope (FE–SEM) was used to investigate the microstructure and the morphology of the films. Elemental depth profiles of the coatings were obtained using a secondary ion mass spectrometer (SIMS). Nanomechanical properties were determined by nanoindentation. Tribological properties of the coatings were studied using "pin-on-disc" testing. Chemical bonding was investigated by Fourier transform infrared spectroscopy (FTIR). Nanostructure and crystallinity of the films were evaluated by transmission electron microscopy (TEM) observations. Spectrophotometer has been used to measure the optical transmittance and reflectance of the films over the spectral range from 280 to 1000 nm. The effect of the deposition parameters on the wear-resistance, mechanical, optical and optoelectronical properties were discussed.

NANO-COMPLEXES DNA / CATIONIC BIODEGRADABLE POLYMERS FOR POTENTIAL APPLICATIONS IN GENE THERAPY

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The development of efficient and safe gene delivery carriers has been a major challenge in the clinical application of non-viral gene therapy. Recently, cationic polymers (CPs) are of increased interest to be used both, in gene therapy [1 – 3] and biotechnology [4, 5]. Herein, we report novel biodegradable highly charged CPs on the basis of naturally occurring building blocks, such as amino acid arginine and endogeneous multi-amine spermine. To render CPs biodegradable, we synthesized various cationic polyamides and polyureas *via* an original one-pot synthetic strategy [6], which are able to hydrolyze (biodegrade) in physiological environment with releasing free spermine utilizable by the organism.

The new CPs revealed a high *in vitro* cell compatibility within the concentration range 0.04 – 10.00 mg / mL (evaluated using mammalian cell lines, including 4T1 (murine mammary carcinoma), HeLa (human cervical adenocarcinoma), NIH3T3 cells (mouse fibroblast) & CCL 210 (human fibroblast). Further, the new CPs were highly water soluble (≤ 200 mg/mL) that is important for their practical applications, they formed a positively charged (zeta potentials ≤ + 57.4 mV) stable nanocomplexes with pDNA (38.0 – 312.0 nm) at rather low polymer / pDNA weight ratios (WR = 5/1 – 25/1). The cellular uptake of complexes was evaluated by flow cytometry (FACS) analysis and confocal microscopy study; The new CPs showed selective transfection activity towards certain cell lines that could be promising for practical applications in gene therapy, some of them revealed also rather high activity against bacteria (tested with *Bacillus cereus, Staphylococcus aureus*, *E.coli, Salmonella enterica*) and could be of interest as nontoxic antimicrobial agents for numerous applications.

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ELECTRICAL PROPERTIES OF THE COMPOSITE CELLULOSE–INSULATING OIL–WATER NANOPARTICLES

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The paper presents investigated the dependencies of DC conductivity electrical pressboard impregnated insolating oil of moisture content and electric field strength. The studies were conducted for measuring temperature in the range of 20 to 100 °C and the electric field strength in the range of 10 to 1000 kV / m. With approximate waveforms in double logarithmic coordinates conductivity depending on the intensity of the electric field exponential function determined coefficients of determination R^2. The value of this ratio is close to unity, which provides high accuracy measurements of conductivity and the exact stability and temperature measurements. It was found that the influence of the electric field E on the DC conductivity is described exponential dependence exp $(E\,d / k\,T)$.

This research was partially funded from the statute tasks of the Lublin University of Technology, at the Faculty of Electrical Engineering and Computer Science, 8620/E–361/S/2016 (S–28/E/2016), entitled “Researches of electrical, magnetic, thermal and mechanical properties of modern electrotechnical and electronic materials, including nanomaterials and electrical devices and their components, in order to determination of suitability for use in electrical engineering and to increase the efficiency of energy management”.

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Dr.ph ZAUR BERISHVILI

Planar Magnetron Spraying Apparatus

WIPO PCT/GE 2016000005 *C23C 14/35 (2006.01)* 26 April 2016

Nanotechnology: Nanofilms Deposition