МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ ДВНЗ «Прикарпатський національний університет імені Василя Стефаника» Кафедра фізики і хімії твердого тіла Фізико-хімічний інститут Навчально-дослідний центр напівпровідникового матеріалознавства Державний фонд фундаментальних досліджень АКАДЕМІЯ НАУК ВИЩОЇ ШКОЛИ УКРАЇНИ НАЦІОНАЛЬНА АКАДЕМІЯ НАУК УКРАЇНИ Інститут фізики напівпровідників ім. В.Є. Лашкарьова Інститут фізики напівпровідників ім. В.Є. Лашкарьова Інститут металофізики ім. Г.В. Курдюмова Інститут загальної і неорганічної хімії ім. В.І. Вернадського Українське фізичне товариство Інститут інноваційних досліджень

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Materials XVII INTERNATIONAL FREIK CONFERENCE ON PHYSICS AND TECHNOLOGY OF THIN FILMS AND NANOSYSTEMS

MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE Vasyl Stefanyk Precarpathian National University Physics and Chemistry of Solid State Department Physical-Chemical Institute Educational Research Centre of Semiconductor Material State Fund of Fundamental Research ACADEMY OF SCIENCE OF HIGH SCHOOL OF UKRAINE NATIONAL ACADEMY OF SCIENCE OF UKRAINE V.E. Lashkarev Institute of Semiconductor Physics Chuiko Institute of Surface Chemistry G.V. Kurdyumov Institute of the Physics of Metals V.I. Vernadsky Institute of General and Inorganic Chemistry Ukraine Physics Society Institute of innovation research УДК 539.2 ББК 22.373.1

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Представлено сучасні результати теоретичних і експериментальних досліджень з питань фізики і технології тонких плівок та наносистем (метали, напівпровідники, діелектрики, провідні полімери; методи отримання та дослідження; фізико-хімічні властивості; нанотехнології і наноматеріали, квантово-розмірні структури, наноелектроніка, тощо. Матеріали підготовлено до друку <u>Програмним комітет</u>ом конференції і подано в авторській редакції.

Для наукових та інженерних працівників, що займаються проблемами тонкоплівкового матеріалознавства та мікроелектроніки.

Рекомендовано до друку науково-технічною радою Фізико-хімічного інституту ДВНЗ «Прикарпатський національний університет імені Василя Стефаника»

XVIII International Freik Conference Physics and Technology of Thin Films and Nanosystems. *Materials.* / Ed. by Prof. V.V. Prokopiv. Ivano-Frankivsk : Publisher Vasyl Stefanyk Precarpathian National University, 2021. 202 c.

The results of theoretical and experimental researches in directions of the physics and technology of thin films and nanosystems (metals, semiconductors, dielectrics, and polymers; and methods of their investigation; physic-chemical properties of thin films; nanotechnology and nanomaterials, quantum-size structures; thin-film devices of electronics, are presented. The materials preformed for printing by Conference's Organizational Committee and Editorial Board, are conveyed in authoring edition.

For scientists and reserchers on the field of thin-film material sciences and nanoelectronics.

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PLENARY SESSIONS



Develpment of highly efficient bismuth telluride based thermoelectric microconverter

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The flash evaporation method was used to fabricate high-performance p- and *n*-type Bi_2Te_3 -based thermoelectric (TE) thin films. Optimized technological conditions of film preparation, as well as subsequent annealing, give the possibility to achieve a significant improvement in the TE properties of the designed TE films, which are state-of-the-art compared with bulk materials. Furthermore, a brand-new sandwich-layered design of the flexible film thermoelectric microconverter (FTEM) is offered here through the use of perforation cuts between p- and n-legs and a flexible polyimide substrate. Such a unique design makes it possible to avoid a rise in electrical resistance due to an increase in the number of elements in the microconverter. The dimensionless effective figure of merit $ZT \approx 0.6$ (including losses due to parasite heat flux along with the substrate, radiation, and conversion) and TE efficiency $\eta_{max} \approx 3.4\%$ were achieved for the FTEM prototype at the temperature difference ΔT of 100 K ($T_c = 300$ K). Therefore, the use of flash evaporation technology offers the possibility to produce large-scale film TE devices with high efficiency. Moreover, the applicability of the developed FTEM is demonstrated for a thermal detector with a high output voltage, which is used to determine a weak heat flux up to $\sim 10^{-7}$ W.

Density-of-states determination in organic thin-film semiconductors for OLED applications: experiment and theory

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The width of the Density-of-States (DOS) (σ), which is a measure of the energetic disorder in a material, plays a central role in controlling charge-carrier transport properties in organic thin-film amorphous semiconductors, since the charge-carrier mobility changes in an exponential manner with σ : $\mu \propto exp(-(\sigma / kT)^2)$. The experimental determination of the DOS, however, is far from trivial. Several experimental techniques are used to probe the DOS of organic films, such as temperature-dependent SCLC, UPS, inverse photoemission spectroscopy, Kelvin probe force microscopy, as well as thermally stimulated luminescence (TSL). A clear advantage of TSL is that it is a purely optical and electrode-free technique.

In this work we apply the low-temperature fractional TSL technique to determine the DOS of pristine amorphous films of OLED host materials. The DOS width is determined for two series of hosts, namely, (i) carbazole-biphenyl derivatives: CBP, mCBP, and mCBP-CN, and (ii) carbazole-phenyl derivatives: mCP and mCP-CN. We find that the intrinsic DOS can be approximated by a Gaussian distribution. The DOS profile broadens with increasing molecular dipole moments, in a similar manner within each series, in line with the dipolar disorder model. The same molecular dipole moment, however, leads to a broader DOS of CP compared with CBP derivatives. Using QM/MM Molecular Dynamics simulations, we attribute the difference between the series to a smaller polarizability of cations in CP derivatives, leading to weaker screening of the electrostatic disorder by induction. These results demonstrate that the low-temperature TSL can be used as an efficient experimental tool for probing the DOS in OLED materials.

This work has received funding from EU Horizon 2020 Program through the Marie-Curie ITN 'TADF*life*' grant (GA no. 812872).

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Optimization of the characteristics of magnetic field sensors based on magnetic transistor structures

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It is known that the most important quality indicator of magnetotransistor structures (MTS) used as magnetic field sensors is the magnetic field resolution, which is determined by the current transfer coefficient, conversion efficiency and the value of the residual signal. Optimization of MTS can be achieved, in particular, by choosing the initial semiconductor structure (single crystal, epitaxial structure, silicon-on-insulator structure).

The conversion efficiency, as studies have shown, grows with a decrease in the lifetime of minority carriers and with an increase in their effective mobility, and the current transfer coefficient - with an increase in the diffusion length. These parameters should be considered as determining when choosing a material for MTS.

An increase in carrier mobility unambiguously results in an increase in both the transmission coefficient and the conversion efficiency.

We have shown the possibility of creating horizontal drift two-collector magnetotransistors (DMT) based on indium antimonides and experimentally found that they have an S_R conversion efficiency more than an order of magnitude higher than silicon samples of the same geometry. In contrast to the previously known injection magnetosensitive structures based on InSb-madistors, DMT have a significantly better linearity of conversion. The technological method developed by us for increasing the carrier lifetime in *p*-InSb by more than two orders of magnitude due to the diffusion of sulfur at a temperature of 20-25 ° C allows, respectively, increasing the transfer coefficient, and hence the absolute sensitivity of the structures.

The choice of the conductivity type of the starting material is predetermined by the choice of the physical mechanism of magnetosensitivity, which is preferred when creating the sensor. Since the conversion efficiency is also determined by the intensity of the accelerating field, it is obvious that to reduce the sensor current consumption it is advisable to use materials with the highest resistivity.

The baric coefficient of CdSe quantum dot with a three-layer ZnS/CdS/ZnS shell

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Surface passivation of QD due to the use of shell of different materials, proved to be an effective approach to reduce surface defects, which can expand the spectrum of absorption, accelerate the transfer of current carriers and reduce recombination losses. A special positive effect can be achieved if you use the multilayer shell. The QDs are sensitive to deformation, so they are used as sensors of mechanical stress, to study and control the physical characteristics of nanomaterials [1]. The influence of pressure on the physical properties of QD is also related to surface conditions (type of shell, its thickness and number of layers). Additional pressure can be created by adsorbed atoms on the surface of the QD (for example, when interacting with drugs), impurities that alloy the QD, or an acoustic wave. In this work, within the model of the deformation potential, the baric dependences of the energy structure of CdSe quantum dot with a multilayer ZnS/CdS/ZnS shell are calculated. In the assumption of the absence of interaction between quantum dots that have a spherical shape and the same size, the dependence of the baric coefficient of the energy of the radiative transition in quantum dot on the value of the energy, the geometric sizes of the QD core and individual layers of the shell is found.

External pressure leads to shift the edges of the allowed bands, thereby changing the energy spectrum of electrons and holes and the width of the band gap E_g [1]. Thus, the baric coefficient *K* for CdSe QD with a multilayer ZnS/CdS/ZnS shell is determined by three components:

$$K = \frac{\partial E_{00}^{(e)}}{\partial P} + \frac{\partial E_{00}^{(h)}}{\partial P} + \frac{\partial E_g}{\partial P} ,$$

where $E_{00}^{(e,h)}$ is the energy of electron or hole in the ground state.

Under certain conditions (when the hydrostatic pressure exceeds some critical value), the value of the baric coefficient changes (the nonlinear dependence of the radiation energy of QD on the value of the pressure appears).

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Self-organization and formation of ion-induced structures on (100) PbTe crystal surfaces sputtering with Ar⁺ ions

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As is well known, self-organization is a widespread phenomenon and leads to the spontaneous emergence of macroscopic ordering in various systems. In the process of solids sputtering with ion beams, in particular, selforganization can lead to the formation of well-ordered ripples and short-range hexagonally ordered arrays of nanoscale dots. In this report, we discuss another type of self-organization that leads to spontaneous faceting of the lateral facets of ion-induced pyramidal nanostructures which we observed under sputtering of the PbTe crystal surfaces of (100) crystallographic orientation [1].

Our investigations showed that the surface of the PbTe crystal bombarded with Ar⁺ ions is covered with various surface structures and dimples of surface relief. One of the important types of the occurring surface structures is truncated cones covered with protective shield. During sputtering they transform to the cones with pyramidal apexes. The portion of the pyramidal apex increases in the process of sputtering, the portion of the conical base decreases and the cone is gradually transformed into the pyramid. Depending on the orientation of the sputtering surface different regular shapes of pyramidal structures can form, such as trihedral, tetrahedral pyramids or prism-shaped structures placed on the edge with bases inclined to this edge. In addition to the conical-pyramidal transformations, another pronounced feature of the conical-pyramidal topology of PbTe sputtered surfaces occurs, namely the formation of expressive ripplelike patterns on facets of the ion-induced pyramids. The ripples on the different facets of the pyramid have a steady tendency to a conforming location. The wave vector of ripples is perpendicular to the projection of the ion beam onto the pyramid surface planes.

Ion-induced pyramids on the vertices of cones formed on (100) sputtered PbTe surfaces have a tetrahedral shape and are oriented around crystallographic directions [100]. But the orientation of their lateral facets does not coincide with any crystallographic plane of PbTe. Taking this into account we attribute the shaping of such ion-induced pyramids and formation of the well-ordered ripples on their facets to the processes of self-organization involving the contribution of {111} and {110} crystallographic planes of PbTe crystals in the formation of pyramidal facets.

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ORAL REPORTS

Session 1 Thin films technology (metals, semiconductors, dielectrics, conductive polymers) and their research methods



The dependence of energy on the QD deformation and polarization charges

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Recently much attention has been paid to the physics of low-dimensional semiconductor structures. This has been stimulated by the rapid progress in nanometer-scale fabrication technology. Among them, quantum dots, which are also defined as nanocrystals and microcrystallites, or nanoclusters, are of particular interest. The effect of quantum confinement on the electrons and holes in semiconductor QD's has been studied in [1-3].

As in massive semiconductors as in quantum dots optical excitations can lead to exciton states. Real structures can contain various defects. Therefore, conditions may change. For heterosystems in which there is a large difference between the dielectric constants, the effect of polarization charges will be significant. The change in the dielectric properties of the matrix taking into account the polarization or deformation charges leads to a significant change in the energy of both the electron and the hole.

In view of this, in our work we have been calculated the energies of the electron and the hole in the singleband and multibandband (with large, small and intermediate spin-orbital interaction) approximation in the standard form, the energy during deformation or polarization. And we also have been calculated the energies with account both the QD deformation and polarization charges on the QD-matrix interface.

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Understanding of van der Waals forces in thin films of twodimensional materials

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Van der Waals (vdW) forces play a crucial role in biology, physics, chemistry, and form a driving force in the formation of complex twodimensional (2D) multi-layered functional. While, the vdW forces responsible for device stability and interactions at its surfaces, the origin of those forces, has a limited understanding to the date. Therefore, established microscopic longrange vdW forces measurement in 2D stacks, showed vdW attraction long ranges exceeding classical expectations, demonstrate high sensitivity to thin films of water, and weak interlayer couplings between the layers in fabricated stacks. While graphene alone screens vdW attraction forces¹ or show partial transparency in water contact experiments²⁻³, we demonstrate that at greater separations this effect is minor, however, the fabricated graphene stacks may restore graphite-like long-range vdW attractions only in 20 multi-layers. It contrasts to conventional Lennard-Jones predictions and reveals the strongly many-body nature of vdW interactions in 2D materials supporting earlier experiments⁴, and suggesting that attractive mechanism can be associated with quantum mechanical effects, being important in the development of new functional materials and devices.

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New Method of Poling Thin Films of Side-Chain Nonlinear Optical Polymer in Corona Discharge

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Poling of nonlinear optical (NLO) polymers is normally performed at poling temperatures higher than the glass transition temperature T_g of the host polymer. However, some materials start to decompose before their T_g is reached [1].

We propose a novel method for poling NLO polymers at temperatures lower than T_g in the solid state. High mobility of polymer matrix and chains necessary for alignment of the dipoles is provided by the artificial lowering of the T_g . The samples are poled in corona while they are still in a viscous state, or even during their spinning from solution. Thus, the solidification occurs in the electric field provided by corona ions.

The method was tested at the copolymer of methyl methacrylate and 4-(methacryloyloxypropoxy)-4'- nitrostilbene having T_g about 70°C in the solid state. Cyclopentanone was used as a solvent.

We modified a photoresist spin coated for our experiments by insulating the chuck, connecting the electrometer to measure poling current, and placing a specially designed corona triode [2] over the spin coater. Microscopic glass slides with evaporated Al electrodes were used as substrates. Films of the NLO polymer of about 20 µm thickness were spinned from solution.

Kinetics of the solidification at room temperature was measured by monitoring the electric conductivity and the weight of the samples. After initial sharp decrease of both parameters due to evaporation of the solvent, the steadystate condition of the solidification was reached in about 1 h. During all this time, a negative corona was applied. In some samples we observed remarkable decrease of the poling current in 50-60 min indicating probably that poling is completed. Quasi-static pyroelectric coefficients and Thermally Stimulated Depolarization currents were measured in order to evaluate the poling efficiency.

It has been found that the position of the T_g peak at the TSD current curve depended on the storage time of the poled samples gradually increasing from 54°C to 68°C. Relatively high values of the pyroelectric coefficient of about 2 C/m²K were observed clearly indicating that the side-chain dipoles were properly aligned during poling. The method can be recommended for poling other NLO polymers with the relatively high glass transition temperature.

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Optimal Parameters for Corona Poling of Dielectric Thin Films

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Corona poling, especially its modification called the corona triode with the control grid placed between sample surface and corona electrode, is commonly used in the field of electrets, ferroelectric polymers, nonlinear optical polymers and other dielectric thin films for creating the residual polarization in them [1]. Nevertheless, selection of main parameters such as corona voltage, grid voltage, the point-to-grid distance and the grid-to-sample distance is rather subjective and not sufficiently grounded. In some cases, a poorly controlled point-to-plane modification of corona poling is still used. To obtain additional information in this respect, we performed the following three series of measurements.

1. Corona voltage dependence of the surface potential (without a grid);

2. Voltage acquired by a grid at different corona voltages;

3. Current-voltage characteristics of corona at different grid voltages.

Considering the obtained results, we made several suggestions on selection of appropriate corona and grid voltages and formulated limitations of the corona method. In the case of the point-to-plane geometry without a control grid, the sample acquires a definite potential that does not depend on the sample thickness and poling time (in the ranges of 40-150 μ m and 1-60 s). The surface potential in this case is 7 to 10 times smaller than the corona potential.

The onset of corona starts at 4.5-5 kV, so the corona voltage V_c must not be lower than this value. If a grid is used with the grid voltage V_g , then the $V_c > V_g + 5$ kV condition must be fulfilled.

To increase poling current one must use the high corona voltage. However, the power of the grid is limited in this case by the voltage acquired by the grid. For example, at -12 kV the grid voltage cannot be lower than the acquired value of -820 V. At lower corona voltages of 8-10 kV the acquired grid potential is smaller (200-400 V), however the current does not depend on the V_g .

The upper limit of the grid voltage is about 4-5 kV, because at higher voltages the grid itself becomes a source of the corona discharge, so the corona triode does not operate properly any more. The range of applicable grid voltages depends on the corona voltage increasing from 200-1000 V at 6 kV to 400-4000 V at 9 kV. From this point of view, the corona voltage of 9-10 kV can be considered as optimal. However, the power of the grid in this case is low. Therefore, suggested corona voltage is in the range of 10-20 kV depending on the grid voltage.

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Effect of film photocatalyst ZnO:Ho (5 at.%) on the degradation of toluene in air under UV irradiation

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Air purification from the volatile toluene compound, which is a part of many substances used indoors and outdoors, is currently a very urgent problem that attracts the attention of many researchers. One of the most progressive methods for solving this problem is considered to be the method of photocatalytic decomposition of molecules of a pollutant in the medium. The study of such a process is hindered by the strong adhesion of toluene to any surface, which is associated with its high boiling point of 110 °C [1]. In the present work, the elimination of this effect is carried out by carrying out the photocatalytic degradation of toluene at a temperature above 110 ° C, when its adhesion is insignificant.

As a photocatalyst, we used a nanoscale film of the composition ZnO: Ho (5 at.%) 125 nm thick, deposited by explosive electron-beam evaporation. The properties of the film are described in [2]. Photocatalytic decomposition of toluene on the film was stimulated by irradiation of a UV lamp with a maximum at a wavelength of 275 nm. The change in the toluene content was estimated spectrophotometrically at the wavelength of the toluene absorption maximum of 208 nm. The temperature of the air with toluene in the reactor was 112 °C.

The figure shows the dependence of the change in the concentration of



toluene in the air of the reactor under the influence of temperature (1), temperature and photocatalysis (2), only photocatalysis (3). Curves (1) and (2) were measured experiment-tally, curve (3) was determined by the calculation method by subtracting the con-centration values on curve (2) from curve (1).

It can be seen from the figure that irradiation with UV light accelerates the decrease in the concentration of toluene due to its photocatalytic degradation. The kinetics of the concentration change for all curves is close to the kinetics of the first-order reaction $C = C_0 e^{-k\tau}$.

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Smoothing of graphically presented experimental data

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Often the graphical representation of the experimental data, presented in the form of a table, reveals a significant difference in the experimental values of the expected smooth functional dependence, which, according to the researcher, should not be. Based on this, a conclusion is made about significant experimental errors or oscillations. However, if the theoretical functional dependence is known or assumed, then its use confirms or refutes the monotonic or oscillatory nature of the curve. There are numerous applications of smoothing, which is performed primarily to make of data (x-ray pattern, EXAFS, IR spectroscopy et al.) appear to be less noisy than it really is.

Fitting the theoretical curve to an experimental values, we obtain the values of the dependence parameters, which are usually more important than the experimental data, because they generalize them. However, if an expected or predicted curve is absent, the approximation is performed by an arbitrary smooth dependence, the parameters of which do not carry special information or at best information about local characteristics, position and value of the maximum value, if such values are successfully introduced into the functional dependence [1,2].

In the case of the expected smooth dependenceo of experimental results has been proposed to present the processed experimental values with reduced scatter or to smooth. The proposition is based on the following statement: close values of an argument correspond to close values of a smooth function.

Suppose we have a set of experimental points \mathbf{r}_i (x_i , y_i), $i = 1 \dots n$. Improved values, taking into account the values of neighbors, are found by varying the offset $\varepsilon_i = y_i - z_i$ so as to reduce the sum of normalized scalar products of vectors or cosines of the corresponding angles that beginning from the point \mathbf{r}_i and ending at adjacent points \mathbf{r}_{i-1} and \mathbf{r}_{i+1}

 $\mathbf{S} = \sum_{i=2 \dots n-1} (\mathbf{r}_{i,i-1} \ \mathbf{r}_{i,i+1}) / (|\mathbf{r}_{i,i-1}| \ |\mathbf{r}_{i,i+1}|).$

Then, for grafics smoothing we minimize S by increasing from zero to predefined allowable possible values of corrections $|\epsilon_i|$.

This smoothing does not impose smoother course of experimental data dependence by artificially but to detect their hidden smooth nature. Thus, the smoothing result discover a more accurate representation of the physical models.

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Sensory structures based on nanocomposite materials grown on laser technology

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One of the most promising areas of modern solid-state nanoelectronics is the industry, which is based on specific physical effects characteristic of low-dimensional instrument structures - two-dimensional, one-dimensional and zero-dimensional. Among the promising areas of modern nanoelectronics is the development of low-dimensional structures using nanosized composite films related to wide-band semiconductors [1, 2].

The study of the nanostructured state of oxides is defined as one of the most relevant areas of modern semiconductor physics, materials science and electronic instrumentation. Morphological change of such structures contributes to the modification of their optical and electrophysical properties, as well as the emergence of new characteristics that are not inherent in bulk semiconductors. Oxide materials have a wide range of applications as a basis for photovoltaic solar energy converters, LEDs, sensor elements, thin film transistors, color displays.

The most interesting as electrically conductive composite materials are films of oxides ZnO, SnO, InO, etc., which are characterized by a fairly large ratio of surface area to volume. Structuring thin conductive films makes it possible to obtain materials with a wider range of characteristics. One of the most interesting and promising thin conductive oxides of this class is zinc oxide, which is widely used to create transparent conductive electrodes and anti-reflective layers in photovoltaic cells.Zinc oxide is characterized as a material with a wide band gap of ~ 3.3 eV. Due to its thermal, chemical and mechanical stability, it is a promising candidate for use as a source of auto-electronic emissions. The exciton binding energy is 60 mEV.

Zinc oxide crystallizes in three forms: hexagonal wurtzite, cubic sphalerite and cubic modification of the rock salt type. The most common form of ZnO is wurtzite. From the crystal structure of zinc oxide wurtzite follows the presence of zinc oxide piezoelectric properties.

Zinc oxide occupies an important place among wide-gap semiconductors, which are intensively studied due to a wide range of valuable properties and wide application in various industries, military, engineering and medicine. This determines the scientific and applied relevance of the problem - the development and implementation of new technological approaches to the manufacture of instrumental functional structures based on structured oxides, in particular zinc oxides. The solution of these problems requires a thorough study of the nature of physical processes in these structures, new approaches to technologies for their manufacture, including plasma, high-energy and laser, as well as methods of their study.

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Lead Telluride–Based Solid Solutions: ab initio Calculation of Properties

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Thin-film semiconductor devices are relatively cheap and convenient for energy converting and generating. Modern development of production and heat treatment technologies allows to obtain thermoelectric elements with stable operating parameters. The formation of solid solutions from binary compounds or the introduction of impurities of other atoms into the crystal lattice is widely used to improve the functional parameters of the manufactured devices.

PbTe-based thin film micromodules can be used in miniature devices or flexible systems for thermoelectric energy harvesting. The widespread implementation is due to the high efficiency and quality as thermoelectric and detector materials [1]. Their production, compared to bulk materials, is more convenient due to the use of a much smaller amount of raw material, and, in addition, the values of thermoelectric figure of merit are much higher. Solid solutions based on PbTe are quite promising compounds due to the possibility of forming on their basis both homogeneous materials with low doping content and the formation of nanoinclusions in the basic material.

Ab initio calculations of equilibrium positions of atoms in a cluster, distribution of electron density, total energy, frequencies and oscillation spectra of ternary compounds on the basis of lead chalcogenides are carried out using Becke-Lee-Yang-Parr exchange-correlation functional (B3LYP) and Stevens-Basch-Krauss-Jasien-Cundari (SBKJC) basic set.

Ab initio methods are quite sensitive to the components of the studied structures. When one of the Pb atom is replaced by Cd, Sn or Ge atom, the change in the thermodynamic parameters in the cluster of 64 atoms is already significant [2]. For example, for the basic PbTe compound, with replaced the inner metal atom, there was an increase in thermodynamic parameters in a wide temperature range (20-1000 K).

This study was supported by the Ministry of Education and Science of Ukraine as the project for young scientists "Technology of thin-film thermoelectric micromodules based on multicomponent compounds with quantum-size effects" (0119U100062).

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Multilayer indium saving ITO thin films deposited by DC sputtering method on preheated glass substrates

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Indium tin oxide thin films have been extensively studied due to their applications as transparent electrodes for solar cells, at panel displays and for optical solar reflectors because of their low resistivity and high transmittance. However the great disadvantage of usage of indium in thin films fabrication is it high price. In order to find a material that is more cost effective, has better or maintains properties of conventional ITO (90 mass% In₂O₃ and 10 mass% SnO₂) (ITO90) ML thin films consisting of very thin layer of conventional ITO and indium saving ITO (50 mass% In₂O₃ and 50 mass% SnO₂) (ITO50) layer were deposited onto glass substrates preheated at 523 K by DC sputtering.

Results of X-Ray 2θ scans reveal that as-deposited ML ITO90/ITO50 thin films show polycrystalline structure.

Cross-sectional TEM images of the ML ITO90/ITO50 thin film with 150 nm thickness clearly demonstrate two layers. The first layer is about 14 nm thick and the second layer thickness is about 136 nm. The second layer shows the columnar vertical growth.

It was revealed that at the optimum oxygen flow rate the volume resistivity of as-deposited ML ITO90/ITO50 films is lower (281 $\mu\Omega$ cm) than that of SL ITO50 films (714 $\mu\Omega$ cm).

Optical transmittance of ML ITO90/ITO50 thin films deposited at optimum oxygen flow rates $Q(O_2)=0.3$ sccm and $Q(O_2)=0.5$ sccm reaches 98.3 and 97.1% at $\lambda=550$ nm, respectively.

Roughness of ML ITO90/ITO50 thin films is significantly lower than that of SL ITO90 thin film with the same thickness.

Morphology of island structures formed by self-organization processes during melting of lead films

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Arrays of metal nanoparticles have a wide range of spheres for applied use. To obtain them, along with chemical technologies, the methods based on thermal dispergation of thin films are widely used. However, many issues of such processes still require specification.

The given work is devoted to the study of the morphology of island structures formed during the melting of continuous polycrystalline films of lead on the amorphous carbon substrate. Pb/C samples with a lead layer thickness from 15 to 300 nm were being obtained by the method of samples of variable composition by the way of vacuum condensation of components. The films were condensed onto the substrates at the room temperature, and after condensation completion, they were briefly annealed in a vacuum at the lead melting temperature. Obtained samples were studied using a SEM (Tescan Vega 3).

It is shown, that due to self-organization during lead melting, an array of spherical metal particles is formed on the substrate. Herewith, the de-wetting of initially continuous polycrystalline lead films occurs in several stages. Initially, as the temperature rises, the continuous film, being still in the solid phase, decays into islands of an irregular surface shape. During further heating, the islands completely melt, acquiring the typical shape of the spherical segment.

The size dependences of the substrate coverage with a film, the number and the most probable radius of particles formed during the films melting, and the full width at half maximum of the histograms of their size distribution were obtained. It is shown, that all size dependences have a break at the mass thickness of the initial films of about 100 nm. The observed behavior of the size dependences is explained by the change in the morphological structure of the initial film upon reaching this critical thickness.

Thus, for example, films, the thickness of which is bigger than the critical one are initially continuous polycrystalline. Their decay turns out to be energetically favourable and is due to the excess energy connected with various defects of the vacuum condensate. Estimates show that the energy of the intergranular boundaries, which are the main defect in a polycrystalline film, is an initiating factor of the thermal dispergation. It is the polycrystalline structure that determines the kinetics of the decay of initially continuous films. At the same time, thinner samples consist of separate and, probably, single-crystal islands that do not have thermodynamic stimuli for further decay. When heated, such particles only change their shape, gathering into spherical drops, but practically do not experience further decay.

Defect formation in oxygen-doped cadmium telluride thin films

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Operation of photoconverters under harsh conditions (e.g., solar concentrators) requires replacing conventional silicon cells with diodes based on other materials. From this point of view, barrier structures of various types, the active region of which is CdTe, are promising due to a special complex of physicochemical properties. The parameters of CdTe can be significantly improved by doping the material with isovalent impurities, in particular, oxygen.

CdTe films grown in oxygen show higher carrier lifetime and lower carrier density, achieving a better performance than devices without oxygen [1].

Oxygen replaces tellurium in the crystal structure of CdTe, which leads to a change in the effective bond charge and, consequently, to additional generation of intrinsic acceptor defects. To analyze defect formation in CdTe:O films, we have used a method of modeling via quasi-chemical reactions, which was successfully applied to describe the defect subsystem of pure CdTe [2].

Since a low diffusion barrier suggests that oxygen can easily reach native defects to form complexes, an assumption has been made about the formation of a complex $(O_{Te}V_{Cd})^{2^-}$. The following quasi-chemical equations have been proposed to describe the formation of impurity defects in CdTe:O:

$$\frac{1}{2}O_2^v = (O_{Te}V_{Cd})^{2^-} + 2h^+ \qquad K_1 = [A^{2^-}] \cdot p^2 \cdot P_{O_2}^{-1/2}$$
$$\frac{1}{2}O_2^v = O_i^{2^-} + 2h^+ \qquad K_2 = [O_i^{2^-}] \cdot p^2 \cdot P_{O_2}^{-1/2}$$

The proposed model has been used for numerical calculations of the concentration of free charge carriers and atomic defects in CdTe:O depending on the thermodynamic parameters.

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Defect formation in tin telluride thin films grown from the vapor phase

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A quasi-chemical model of the formation of intrinsic point defects in tin telluride thin films during their growth from the vapor phase by the hot wall method has been proposed under the assumption of the formation of doubly charged Schottky defects.

Analytical expressions have been obtained for determining the concentration of holes p, tin $[V_{Sn}^{2-}]$ and tellurium $[V_{Te}^{2+}]$ vacancies in terms of the constants of quasi-chemical reactions of their formation and the partial vapor pressure of tellurium.

It has been found that with an increase in the substrate temperature at a constant evaporation temperature, the concentration of holes decreases, which is in qualitative agreement with the experiment [1]. Nevertheless, the calculation of the concentration of point defects has shown that tellurium vacancies V_{Te}^{2+} accumulate in SnTe thin films in an insignificant amount, and the concentration of charge carriers is determined mainly by the concentration of tin vacancies V_{Sn}^{2-} .

An increase in the evaporation temperature at a constant substrate temperature leads to an increase in the hole concentration. In this case, the concentration of tellurium vacancies $[V_{Te}^{2+}]$ and electrons *n* decreases, while the concentration of tin vacancies $[V_{Sn}^{2-}]$ increases.

A change in the partial vapor pressure of tellurium of the additional source at a constant substrate temperature and evaporation temperature at low tellurium pressure (< 10^{-3} Pa) does not affect the concentration of charge carriers and defects. A further increase in the partial vapor pressure of tellurium leads to an increase in the concentration of holes *p* and tin vacancies $[V_{Te}^{2-}]$ and a decrease in the concentration of electrons *n* and tellurium vacancies $[V_{Te}^{2+}]$. In addition, the region, where the concentrations of charge carriers and defects do not depend on the partial vapor pressure of tellurium of the additional source, expands with an increase in the evaporation temperature. This can be explained by the fact that at low tellurium pressure of an additional source, the tellurium pressure in the system is determined by the evaporation temperature.

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Fractality, Percolation, and Average Order as New Structural and Topological Aspects of Metal-Insulator Phase Transitions in Vanadium Oxides

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The metal-insulator (MIT) in vanadium oxides is well studied and have a long history, a solid theoretical basis, and extensive practical applications.

However, in contradistinction to macroscopic indicators of the MIT as changes in conductivity, transparency, etc. modern methods of investigation (Kelvin probe microscopy and / or near-field IR spectroscopy) allow investigating of the microscopic parameters during the MIT in thin VO2 films such as the shape of metal inclusions in the dielectric matrix.

This paper provides an overview of recent advances and results in this area. Three closely interrelated aspects of the evolution of topology and structure for this type of phase transition are discussed - 1) percolation, with the formation of a rarefied infinite cluster of the metallic phase, 2) the fractality of the shape of an individual inclusion, and 3) average order in the metallic phase. The percolation nature of the increase in conductivity as the dielectric is filled with a conducting phase speaks in favor of a random arrangement of new inclusions. Fractality in this particular case means a certain self-similar "irregularity" and irregular shape of the boundaries of these inclusions. If, for such Euclidean figures, the ratio of the area S to the perimeter P as a function of the linear size D has the form S / P ~ $D^{1.0}$, then in the case of the MIT this indicator in function D is the same for the entire ensemble of inclusions and can reach 1.4. The latter means that large inclusions remain statistically similar to their small predecessors, not only with their individual growth, but also with possible subsequent aggregation. It is also noted that, upon MIT in vanadium oxides, the initially arising conducting phase of rutile is not completely ordered and behaves like a "bad metal" that has lost long-range order. Studies of metallic glasses show that this result is not accidental. The presence of fractal ordering as a variant of the "superstructure" at the level of clusters is always associated with the appearance of average order at the level of atoms - partial ordering within small regions from 0.5 to 2 nm in the absence of long-range order. The paper also discusses the possibility of experimental detection of all three of the above structural and topological characteristics of vanadium oxide in the vicinity of the MIT.

Application of pulse current for producing a composite nickel coating

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Electrolytic coatings application represents one of the methods used for metalwork protection against corrosion and abrasion wear during the operation. One promising method of improvement of coatings performance properties involves composite electrolytic coatings (CEC) technology realized by codeposition of metal substrate and reinforcing dispersed particles of the second phase. Growing interest to composite materials in these days is generated by opportunity for making materials which exhibit unique physicochemical properties. Particular attention is given to CEC comprising reinforcing particles relating to class of super-hard materials such as ultra-dispersed diamond (UDD).

Results of electron microprobe analysis and microlevel-based calculation of effective parameters for CEC evaluation (concentration of dispersed phase in a coating (C_{UDD}), average distance between dispersed phase particles in the coating (\overline{l}), degree of surface fill with dispersed phase particles (ratio between surface occupied with a dispersed phase (S_d) and surface across which particles are distributed (S)) are shown in the Table.

It was find out that composite nickel coatings deposited with use of pulse current were characterized with the more uniform and higher UDD particles distribution density across a coating; degree of surface filling with UDD particles was two times higher than for DC-deposited composite nickel coatings.

Deposition mode				C	C /C	$\overline{1}$
	j, A/m ²	<i>f</i> , Hz	Q	C _{UDD} , mass %	S _d /S, %	μm
DC	100	-	-	2.24	10.8	8.04
Pulse current			2	2.38	11.3	6.64
		50	25	2.66	11.9	5.89
			50	4.45	12.4	4.69

Table Deposition modes effect on UDD deposited particles concentration and distribution in a nickel coating

Application of pulse deposition mode promotes increase of UDD particles concentration in composite nickel coatings from 2.24 to 4.45 mass percentage that results in formation of higher dispersed structure: crystalline grains size goes down from 104 nm to 65 nm.

AlGaN/GaN heterostructures for creating microwave field-effect transistors

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1) The large band gap Eg of trinitride semiconductors provides a large gap in the conduction bands at the AlGaN/GaN heterogran, $\Delta E_c > 0.5$ eV, which dramatically reduces leakage currents through the gate (with increasing molar Fraction, Al ΔE_c increases, for AlN/GaN, $\Delta E_c = 2.0$ eV). The electron density in the 2D channel, $n_s > 1 \cdot 10^{13}$ cm⁻², is an order of magnitude higher than that of GaAS; which is due to both modulated doping of the AlGaN layer and piezoelectric polarization – a positive charge at the AlGaN heterogrange. The saturation rate $v_s > 2.5 \cdot 10^7$ cm / s in large electric fields E in GaN is also higher than in GaAs ; it remains high even when the temperature increases. The electrical breakdown fields in GaN are 8 times higher than in Gaas (33•10⁵ V/cm and 4•10⁵ V/cm, respectively), which, with a large gate barrier, allows you to apply a drain-turn voltage $V_{sd} \sim 100 \div 400$ V. Large n_s values combined with large breakdown fields provide a microwave power density in GaN-HFET 10 times greater than in GaAs – HFET; GaN transistors have high efficiency, a wider frequency range and output impedance. [1].

2) Generation and recombination processes at surface levels in AlGaN/GaN-HFET are weakened due to high E_g values; lower sensitivity to such effects contributes to a decrease in noise levels (HFET with $L_d = 0.1$ microns have a noise level of 0.6 dB). The high thermal conductivity of GaN (1.7 W/cm•K) compared to GaAs (0.53 W/cm•K) and the higher effective electron mass (0.2 m₀ for GaN and 0.067 m₀ for GaAs) provide a lower probability of scattering at elevated temperatures and efficient operation of devices up to 400°C. The achieved picosecond Electron flight times in the submicron channel (L < 1 µm) at High fields are due to the ballistic trajectory of their movement, which occurs due to the absence of electron-phonon scattering (optical phonon energy in GaN $\eta\Omega_0 = 91$ meV, and GaAs $\eta\Omega_0 = 36$ meV). For a GaN HFET with a channel length $L_d = 0.1$ microns, the 100 GHz limit frequency is exceeded. [2].

3) The output volt-ampere characteristic of the GaN-HFET at high ISD currents has a section of negative differential conductivity, which may be caused by the transition of carriers in the GaN from 2D channel to 3D States. The AlGaN/GaN-HFET energy diagram, which differs from AlGaAs / GaAs, allows for the possibility of such transitions [3].

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Development of a technology for low-temperature ion-plasma deposition of nanostructured ALN layers

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Nanostructured films of hexagonal aluminum nitride obtained by high frequency (13.56 MHz) reactive magnetron sputtering of an aluminum target in an Ar i N₂ gas mixture (1:3.5, respectively) at: the working pressure of gases in the chamber is 0,8-2 Pa, the plasma discharge power is 1600 W, and the film deposition rate is 10 - 23 nm / min



Fig. 1 Three - dimensional (3D) image of the surface of an AlN polycrystalline film on an n-Si (111) substrate

Fig. 2 Dependence of the capacitance (1) and tangent of the dielectric loss angle (2) AlN on frequency.

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In Fig.1 shows a three - dimensional (3D) image of the surface of a polycrystalline AlN film on an n-Si (111) substrate. The surface of the AlN film is typical of polycrystals – it is formed from nanocrystalline grains with clear boundaries, which are clearly visible in the form of globular nanomorphology in a three-dimensional image. The characteristic linear grain sizes range from 20 to 100 nm. This indicates that the growth morphology of AlN films deposited by Ion sputtering methods at relatively low temperatures is columnar.

The dielectric properties of AlN films in the manufactured Al/AlN/Si/capacitor structures were also studied. From the obtained results, it follows that the capacitance (permittivity) curve gradually decreases from 10 to 3.5 as the frequency of the electromagnetic field increases from 25 Hz to 1 MHz (fig. 2). At the same time, the tangent curve of the dielectric loss angle passes through a wide maximum with a value of 0.2 near 10 kHz. Such features indicate the existence of orientation polarization of dipoles in the obtained AlN films.



ORAL REPORTS

Session 2

Nanotechnologies and nanomaterials, quantum-size structures



Organic-inorganic nanocomposites for absorption of electromagnetic radiation

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Minimization of the influence of electromagnetic field on humans is of great importance since electromagnetic radiation (EMR) harms living species by affecting bioprocesses at the cell level and injures nervous, immune and other systems. On the other hand, action of EMR on electronic devices results in emerging of spurious signals that may cause malfunctioning of the equipment and lead to partial or even total loss of information. An important problem is protection of electronic communication channels against unauthorized access by acquiring of accompanying electromagnetic radiation [1]. To mitigate the EMR influence and to protect electronic equipment and humans' vital space protective coatings that absorb (reflect and/or scatter) microwaves are greatly desired.

In the present work, formation procedures and properties of organicinorganic nanocomposites based on epoxy polymer matrix containing a mixture of magnetite and polyaniline (PANI) doped with carbon nanotube (CNT) are studied.

It was found that composite containing magnetic micro- and nanoparticles and particles of polyaniline doped with CNT exhibits strong microwave absorption. In the wavelengths range from 1000 nm to 2000 nm spectral distribution of the absorption coefficient $(A, \text{ cm}^{-1})$ for all composites being studied exhibit absorption bands at the spectral interval 1380-1420 nm, 1670-1680 nm and 1900–1950 nm. The highest value of A at 1680 nm is observed for composites containing 5% of nano-dispersed magnetite and 5% PANI-CNT (A =57.2 cm⁻¹). For composite without filler, absorption coefficient amounts only 3.5 cm⁻¹ and 14.8 cm⁻¹ for composites containing only PANI. It was found, that the coating made of composite with highest absorption also possesses the best mechanical properties, in particular, high microhardness. At the same time, prepared thermosetting composition provides not only high microhardness and IR-absorption but effective water protection and excellent anticorrosive properties when used as the coating on the surface of steel [2]. This makes the proposed composite perspective for EMR shielding, for anti-radar purposes reducing the intensity of microwave radiation scattered by a target and at the same time act as protective coatings on the surface of metals.

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Synthesis and optical properties of CuO nanoparticles stabilized by rhamnolipid biocomplex

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Concentrated (up to 10 g/L) colloidal solutions of copper oxide nanoparticles (CuONPs) were synthesized via the decomposition of freshly prepared copper hydroxide in an alkaline medium in the presence of biogenic surfactant (rhamnolipid biocomplex, RBC) synthesized by Pseudomonas sp. PS-17. Using SEM it was found that the obtained CuONPs form agglomerates of irregular shape with a size of 35 - 90 nm. The sizes of crystallites of synthesized CuONPs were calculated by the Scherrer equation using XRD patterns and it was found that the size of the crystallites decreases from 12 to 5 nm with increasing initial concentration of RBC from 1 to 5 g/L. Since the CuONPs is semiconductor of the *p*-type, it's characterized by the phenomenon of surface plasmon resonance that is why the spectral characteristics of obtained solutions were investigated. It was observed that Uv-vis spectra of obtained CuONPs are characterized by intense absorption band at 275 nm and a weakly expressed "shoulder" in the wavelength range 300-400 nm (Fig. 1). However, the absorption intensity of colloidal solutions increases nonlinearly with increasing RBC concentration. This effect can probably be explained as follows.



Fig. 1. Absorption spectra of colloid solutions of CuO, obtained in the presence of 1 g/L (a), 2 g/L (b) and 5 g/L (c) RBC. Insertion is the dependence of the optical density of solutions at 275 nm and 365 nm on the size of CuO crystallites.

According the to Mi' theory, the value of the extinction coefficient of small particles is proportional to their radius and concentration. Besides. the concentration of the particles is inversely proportional to their radius in a cube. Thus, the optical density of the CuONPs solutions must be inversely proportionnal to the square of their size. It was found (Fig. 1, Insertion) that the values of O. D. of obtained CuONPs is inversely proportional to the square of the size of their crystallites.

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Effect of the electric field on the energy states of the acceptor impurity in the GaAs/Al_xGa_{1-x}As quantum dot

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In the field of modern nanotechnology, it is very important to control different properties of nanoonbects with high precision. Ways to solve this range of problems are to change their size, doping and applying external fields.

Different properties (especially optical properties) depend on the impurity position and external fields. The changing of the external field caused changing the probability density of electron location in different shells.

In this work, we study the effect of electric field and acceptor position on the optical properties of $GaAs/Al_xGa_{1-x}As$ quantum dots. The impurity displacement from the spherical quantum dot (QD) center causes splitting electron levels (for excited states). Those impurity displacement also causes the shift of the absorption band into the low-energy region.

For the hole and acceptor states the multiband effective mass models should be used. For considered nanosystem $GaAs/Al_xGa_{1-x}As$ the Luttinger model with spherical approximation comfortably can be used.

In the heterostructure $GaAs/Al_xGa_{1-x}As$, the band gap Eg and the spinorbit interaction Δ_{so} are large. Therefore, for hole and acceptor states multiband models of effective masses should be used. And for $GaAs/Al_xGa_{1-x}As$ heterosystem it is convenient to use the Luttinger model with spherical approximation.

We place the hydrogen impurity at a distance D from the center of the QD. The external electric field F_{el} is applied to the heterosystem and we considered three cases of electric field directions.

As a result of research the spectrum of holes in a multiband model in an electric field is determined. The dependence of the hole energy spectrum on the radius of the quantum dot and the location of the impurity from the center of the quantum dot is shown. The dependence of the energy spectrum of central and non-central acceptor impurity in the electric field and without it is obtained.

Influence of oxygen on structural and electrical properties of CdS (100)

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Today, much attention is paid to alternative and renewable energy. Among such energy sources, the leading place is occupied the solar energy and fuel cells, which are an integral part of alternative energy devices [1]. One such key structure is CdS-based solar cells.

In this paper, the electronic properties of CdS (100) films without impurities and with the addition of O_2 oxygen molecules are investigated, based on calculations from the first principles. We obtained valence electron density distributions and electron energy spectra for the CdS (100) film without impurities and with the addition of O_2 oxygen molecules. Calculations were performed using the author's program code [2].

Our calculations show that the increase in the catalytic activity of the CdS film occurs when the surface Cd atoms are replaced by oxygen atoms. The oxygen concentration ranged from 3.125% to 12.5%. It can be assumed that oxygen, due to its high electronegativity, is adsorbed on the surface of CdS as a negatively charged ion, removing electrons from the surface atoms of the CdS film. Also, we recorded that with increasing oxygen concentration, there is a decrease in the number of free bonds and an increase in the band gap, which leads to a decrease in catalytic activity, degradation of the CdS film and a decrease in photocurrent. According to the calculations for the study of small diatomic and triatomic clusters (S, Cd), we found that the inclusion of oxygen atoms or atoms of other kinds in small clusters (S, Cd) affect the catalytic activity of research systems as a whole [3, 4].

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Changes in the Surface Structure of Silicon with the Natural and Artificially Grown Oxide Due to Ion Irradiation

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The possibility of using fast light and heavy ions to change the morphology and optical properties of the surface of irradiated silicon with different thicknesses of surface oxide for the subsequent creation of surface composites and composite films on silicon substrates was investigated. Such composites in the case of the deposition of nanosized metal inclusions are promising for the creation of modern opto- and nanoelectronic devices based on the phenomenon of excitation of surface plasmons (oscillations) and surface plasmon polaritons (waves).

Our studies of silicon with natural oxide, irradiated with 27.2 MeV helium ions, have demonstrated the specificity of its optical and structural properties at high fluences. Metallographic studies of the structure of irradiated Si reveal the distribution of defects along the direction of irradiation. The results obtained indicate that the highest Si lattice stresses are concentrated in the region of ion deceleration. Nevertheless, at high fluences, a layered distribution of stresses is observed both in the path region of the ions and beyond of their braking line. With such fluences, the polarization ellipsometry method reveals an abrupt change in the absorption coefficient of Si, and experiments involving an AFM indicate a significant increase in surface roughness. These circumstances became decisive for the use of this material in the course of further research.

The thermal deposition of the gold film onto such modified silicon surface leads to the formation of an island film from separate isolated gold grains, whereas on a plane surface under similar deposition of Au, the film acquires a labyrinth structure.

In the case when SiO_2 oxide about 500 nm thick is deposited onto silicon before irradiation, the situation will become somewhat different. Heavy ¹³¹Xe ions with an energy of 130 MeV cause ionization and excitation of the atoms of material along the entire motion trajectory. Herewith, a hidden track is formed that can be detected by chemical etching. The deposition of the gold film on such porous surface and its' further annealing lead to the uneven filling of the pores of the oxide layer with Au nanoparticles. Gold particles are located on the surface of SiO₂ and in the pores of the upper part of the film with a thickness of about 100 nm due to uneven (in sizes) etching of nanopores deep into the SiO₂ film.

Thus, by depositing Au onto the rough surface of Si, previously irradiated with significant fluences of helium ions, or by introducing Au nanoparticles into the SiO₂/Si structure modified with fast ¹³¹Xe ions, it is possible to create surface nanocomposites on a silicon substrate.

Influence of impurity and electric field on the spectral parameters of an electron in a quantum dot - quantum ring semiconductor nanostructure

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The intensive development of nanotechnology has made it possible to create new nanostructures with clear geometric shapes. In particular, at present, structures containing quantum dots and nanorings have been created and are being intensively investigated. The unique properties of quasiparticles in such systems make it possible to use them as basic elements of tunnel nanodiodes, nanotransistors with high electron mobility, high-efficiency light emitting devices, photoelectric converters, optical sensors, nanosensors for diagnostics of various biological and chemical compounds [1, 2].

In this work, we investigate a nanostructure consisting of a cylindrical semiconductor quantum dot (quantum well, GaAs medium), which through a finite potential barrier ($Al_xGa_{1-x}As$ medium) is tunnel-connected to a coaxial cylindrical nanoring (quantum well, GaAs medium). The donor impurity is located on the axial axis of the nanostructure. It creates an attractive Coulomb potential for an electron. A homogeneous electric field with strength *F* is directed perpendicular to the axial axis of the nanosystem.

The calculation of the energy spectrum and wave functions of the electron was performed in the model of effective masses and rectangular potential energies. The stationary Schrödinger equation for an electron interacting with an impurity and electric field cannot be solved analytically exactly. Therefore, the electron spectrum was found by the method of expansion the unknown wave function of a quasiparticle with a complete orthonormal set of electron wave functions in a nanostructure without impurity and electric field and subsequent solution of the obtained secular equation.

The dependence of the electron energy spectrum and the oscillator strengths of intraband quantum transitions on the geometric characteristics of the nanostructure and the magnitude of the electric field strength are theoretically investigated. All these dependences are complicated and non-monotonous, due to the complicated nature of the density distribution of the probability of location of electron which is interacting with impurity in nanostructure.

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Core-shell spherical quantum dot type-II under an external electric field

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The colloidal core-shell QDs are heterostructures that can be obtained by the cheap chemical synthesis technologies. The atom-like spectrum of these nanostructures can be changed by tuning the size of the core and the thickness of the shell. The size of the core and the thickness of the shell control the physical properties of such nanostructures. At quantum dots type II the interband absorption energy is less than the band gap of any of the constituent semiconductors due to the different spatial localization of the charge carrier. The spatial separation of the carriers in QD type-II has a number of useful physical applications.

In this study, we present a simple one-band model within the effective mass approximation to describe the electric field impact on the energy structure and the optical properties of QD type-II CdSe/ZnTe (Fig.1).



The dependences of the energies and oscillator strengths interband quantum transitions on the external electric field strength are calculated by the diagonalization method [1-2]. It is shown that in the absence of an electric field due to spherical symmetry of nanosystem only quantum transitions $\Delta l=0$ are allowed (1s_e-1s_h, 1p_e-1p_h, 1d_e- $1d_h$, $1s_e$ - $2s_h$, ...). The oscillator strength of quantum transitions between the excited states of the electron and the hole is greater than between the ground states. But the spherical symmetry is broken under the influence of the electric field, therefore, the oscillator strength of quantum transitions 1se-1ph, $1s_e-1p_h$, $1s_e-1d_h$, ... increase when electric field strength grows.

It is shown that the exciton lifetime increases with increasing electric field strength due to the

overlap of the electron and hole wave functions

Fig.1. Geometrical and potential scheme QD Type-II CdSe/ZnTe

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Impurity photoionization cross-section and light absorption coefficient in multilayer spherical quantum dots

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Energy spectrum, wave functions and binding energies of the electron to the donor impurity ion located in the center of a multilayer spherical quantum dot (MSQD) consisting of a core GaAs and two spherical shells Al_xGa_{1-x}As and GaAs (Fig. 1) were studied within the effective mass approximation. Based on the exact wave functions of the electron expressed in terms of Coulomb functions of the first and second kind, the spectral dependences of the photoionization cross section of the impurity (PCS) and the intersubband optical absorption coefficient (OAC) for various geometric dimensions of the nanostructure were calculated.



Fig.1. Electron potential energy in MSQD at Z = 1.

It is shown that the decrease in the width of the external potential well changes the localization of the electron in the nanosystem which significantly affects the binding energy of the electron with the impurity, photoionization cross section and absorption coefficient. intersubband The position of the PCS peak associated with the quantum transition of an electron from the ground state to the 1p^o state shifts to the region of higher energies, and its height decreases. At the same time, the height of PCS peaks associated with quantum transitions to higher

excited states (2p⁰, 3p⁰) increases.

The presence of impurities and changes in the MSQD size significantly affect the intersubband absorption coefficient. Decrease of the external potential well width in the absence of impurities leads to a monotonous increase in OAC through the first excited state, and in the presence of a central impurity, absorption through states with higher energy increases.

Obtained results enable prediction of the specifics of the effect of the magnetic field on the optical properties of MSQD with two potential wells. Increasing the induction of the magnetic field reduces the cyclotron radius of the electron rc=eB. If this becomes smaller than the MSQD radius, the magnetic field will increase the confinement and decrease the effective potential well width in the direction perpendicular to the magnetic field.

Peculiarities of electronic structure of silicon nanoparticles obtained by electric-spark dispersion method

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Silicon nanoparticles have been attracting a lot of attention lately as they demonstrate important properties for their technological application as a deoxidizer in steelmaking, alloy manufacturing, in the semiconductor industry, as electrode material for lithium-ion batteries, in optoelectronic devices, etc. Silicon nanoparticles were synthesized by electric-spark dispersion method in water. Peculiarities of electronic structure of silicon nanoparticles were studied by ultrasoft X-ray emission spectroscopy (USXES).



Fig. 1 (a) Si L_{α} -emission spectra: 1 – sample obtained using silicon electrodes in water, 2 – reference semiconductor silicon wafer (c-Si), 3 – reference pyrogenic silicon dioxide (SiO₂).

(b) SEM image of silicon nanoparticles obtained by the electric-spark dispersion method using silicon electrodes and silicon granules in a water.

Shape of the SiLa band of nanoparticles obtained in water (Fig. 1a) is close to the SiLa from silicon dioxide. However, the of the spectrum nanoparticles shows "a" maximum, which appears at the same energies as such feature in c-Si. In addition, the intensity of the subband "a" is higher in the sample obtained with the use of silicon electrodes in

water than in SiO_2 by 1.6 times due to the maximum from silicon. This indicates that the spectrum of the samples obtained using silicon electrodes in water reflects the valence bands of mixtures of pure and oxidized silicon nanoparticles.
The hybridization of the plasmons in the cylindrical metallic nanoshell

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The spectral position of the localized surface plasmonic resonances (SPR), which are excited in the metallic nanostructures, depends on the size and the shape of the structure, on the material of the structure and on the local dielectric environment [1]. Among the different nanostructures the structures of the type "core – shell", with or without the cylindrical ones, attract the special attention. This is due to the more flexible possibilities for the control of their optical properties.

The particularities of the optical properties of the layered structures in the dissipativeless approximation are well explained by the plasmonic hybridization model [2]. The optical response of the complicated nanostructures in the frameworks of this model is the result of the hybridization of SPR, which takes place in the nanostructures of the elementary geometry. Thus, the transverse SPR of the cylindrical metallic nanoshell can be considered as the composition of SPR of the infinite cylindrical dielectric cavity and the infinitely long solid metallic wire

$$(\omega_{sp}^{\perp(\pm)})^{2} = \omega_{p}^{2} \left\{ {}^{\circ}o^{\infty} + \frac{1}{2(1-\beta_{c})} \{ (1-\beta_{c})({}^{\circ}o_{c} + {}^{\circ}o_{m})m \right\}$$

$$m \left[(1+\beta_{c})^{2}({}^{\circ}o_{c} - {}^{\circ}o_{m})^{2} + 2\beta_{c}({}^{\circ}o_{c}^{2} + {}^{\circ}o_{m}^{2} + {}^{\circ}o_{c}^{\circ}o_{m}) \right]^{\frac{1}{2}} \right\}$$

$$(1)$$

where ω_p – the frequency of bulk plasmons in metal of the shell; σ^{∞} – the contribution of ion core; c_a and c_m – the dielectric permittivity of the material of the core and the dielectric permittivity of the environment correspondingly; β_c – the volumetric content of the material of the core in the layered structure.

It should be pointed out that the formula (1) transforms into the known expression [3]

$$\left(\omega_{sp}^{\perp(\pm)}\right)^{2} = \frac{\omega_{p}^{2}}{2} \left[l \pm \left(\frac{a}{b}\right)^{2} \right].$$

$$(2)$$

under $o^{\infty} = o_{c} = o_{m} = 1$ taking into account that $\beta_{c} = (a / b)^{2}$.

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Photostimulated synthesis of decahedral silver nanoparticles

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The development of new methods of metal nanoparticles' and semiconductors' synthesis and further creation of functional materials on their basis is a critical stage in the advancement of nanotechnologies. In recent years, evolution of chemical methods for the nanoparticles' synthesis has enabled a high level of control over their morphology by manipulating the growth kinetics of different crystalline phases.

Despite the fact that photostimulated synthesis is quite popular, there is no information nowadays on the necessary and sufficient conditions for the formation of a certain shaped metal nanoparticles (silver and gold) utilizing photostimulated reactions, besides published results are contradictory.

The investigation carried out by us, showed that the ratio of excitation wavelength energy and plasmon resonance energy E_{ex}/E_{res} depends on the shape of silver particles and is 1.3 ± 0.1 for decahedra and 1.1 ± 0.1 for prisms. The general trend shows that the difference between the excitation wavelength energy and the resonance energy for the formed particles of decahedral shape is smaller than for prismatic particles.



Fig.1 A typical image of silver decahedral nanoparticles, obtained using a scanning electron microscope (left) and the dependence of the position of the plasmon resonance maximum on the excitation wavelength (right).

Controllable hydrothermal synthesis of α and β modification MnO₂ nanostructures for hybrid capacitors application

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Hybrid electrocemical capacitors are perspective direction of electrochemical energy sorcers development due to the high of specific power

and energy. The carbon is the material for a polarized electrode. However. for an unpolarized electrode are reserched the oxides, hydroxides, and sulfides of transition Transition metal metals [1]. oxide. oxide (MnO_2) manganese α and β modification has been one of the most inorganic high-performance attractive electrode materials in consequence of its excellent physical and chemical properties [2].

In this paper we report of the synthesis of $MnO_2 \alpha$ and β modifications (average size of the particles are 14-16 and 15-18 nm respectively). The concentration of KCl 4M is a key factor in the formation of MnO₂ α and β – modification (Fig. 1, a).

The electrochemical properties of α and β -MnO₂ were examined in supercapacitor using cyclic voltammetry. It was determined that the value of the specific capacity is significantly higher of MnO₂ α compared than β modifications of 104 F/g and 40 F/g respectively, at a scan rate of 1 mV/s. The stability of the structure and electrochemical parameters of the obtained MnO₂ has been established.



Fig. 1. The schematic representation of the formation of MnO_2 crystals of α and β modifications (a). Dependence of the value of specific capacity on the scan rate (b).

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Plasmons in the doped single-wall carbon nanotubes to the weaklink approximation

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Recently, the optical phenomena in the carbon nanotubes (CNT) in the neighborhood of the plasmonic resonance have been the subject of the intensive research. In addition, the question connected with the propagation of the surface plasmons in the doped CNT is of great interest. In the case when impurity atoms weakly interact with each other, one can assume that electrons on the surface of CNT move in the field of δ -potentials, generated by impurity atoms. Hence, the question connected with the effect of impurity atoms on the dispersion of the surface plasmons in CNT, which is the subject of this work, is actual.

The initial equation for the analysis is the nonhomogeneous wave equation for the vector potential

$$\Delta \boldsymbol{\mathcal{A}} - \frac{\mathrm{T}}{c^2} \frac{\partial^2 \boldsymbol{\mathcal{A}}}{\partial t^2} = -\mu_0 \mathbf{J} , \qquad (1)$$

which has only one nonzero component $\mathcal{A} = \{0, 0, \mathcal{A}_z\}$.

The walls of CNT are considered to be infinitely thin under the calculation of the plasmonic effects, then for the surface current, one can write down $\mathbf{J} = \{0, 0, J_z\}$, where $J_z(r, z, t) = J_z(z)e^{-i\omega t}\delta(r-R)$, and R – the radius of CNT.

Let us assume that impurity atoms are situated at equal distances from each other and generate the periodic nonhomogeneity of conductivity, which can be defined by the sum of the step functions.

The following dispersion equation for plasmons in the doped CNT has been obtained in the frameworks of the proposed model

$$\omega^{2} = \frac{\omega_{p}^{2}b}{\mathrm{T}} \kappa_{q} \frac{K_{0}(\kappa_{q}R)}{I_{0}(\kappa_{q}R)K_{1}(\kappa_{q}R) + K_{0}(\kappa_{q}R)I_{1}(\kappa_{q}R)} \times \left[I_{0}(\kappa_{q}R) + \frac{2\pi\alpha_{0}}{\kappa_{q}^{2}} \left(\kappa_{q}^{2} - \frac{\mathrm{T}\omega^{2}}{c^{2}}\right)I_{0}\left(\sqrt{\kappa_{q}^{2} - \frac{\mathrm{T}\omega^{2}}{c^{2}}}R\right)\right],$$

$$(2)$$

where b – the thickness of the graphene layer; $\kappa_q^2 = q^2 - \tau \omega^2/c^2$, q – the axial wave number; $I_v(x)$ and $K_v(x)$ – the modified Bessel functions of order v, τ – the dielectric permittivity; ω_p – the frequency of bulk plasmons; α_0 – the maximum value of the conductivity.

Influence of annealing on mechanical properties of amorphous metal alloys of Al-Gd-Ni(Fe)

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Amorphous and nanostructured metal alloys are objects as fundamental research and applied developments aimed at the practical application of these materials in various industries [1]. In many aggressive environments amorphous alloys practically doesn't corrode due to the absence of crystalline defects and intergranular boundaries. Alloying changes their properties: corrosive and temperature resistance, etc. High corrosion resistance on the one hand, and chemical activity in redox processes on the other, makes it possible to use amorphous metal alloys as catalysts in heterogeneous catalysis. However, the optimal physico-chemical properties are observed in nanocrystallized AMAs, in the amorphous matrix of which there are pure Al.

It was also explored mechanical properties of AMA before and after annealing of AMA following composition: Al₈₇Gd₅Ni₄Fe₄ and Al₈₇Y₁Gd₄Ni₄Fe₄ annealed at temperatures determined from DSC-curves: 645 K and 647 K for 15, 30, 45, 60 minutes. Have been observed surface of morphology and its elemental composition of annealed surfaces by Scanning Electron Microscopy with an energy dispersive X-ray microanalysis (Tescan Vega 3 LMU). SEMimages shown that annealing leads to the formation of dense oxide layers. Due to heat treatment in an oxygen atmosphere higher concentration of Y fixed in the near-surface oxide layers in comparison with the concentration inherent in formula.

Also, authors [2] shown that microhardness due to annealing increases, which corresponds to the total formation of nanocrystals, increases to 3.9 ± 0.5 GPa. This is due to the fact that after the first stage of crystallization Al nanocrystals are formed. X-ray structural analysis of samples showed that in all cases the Al lattice period is higher than in pure Al (0.40494 nm), which may indicate the formation of a solid Al(R) solution. The size of Al(Y) or Al(Gd) nanocrystals of 15 and 20 nm leads to an increasing of microhardness. The simultaneous presence of Y and Gd inhibits the growth of nanocrystals to a size of 9 nm, which leads to an increasing of the free volume in the amorphous matrix and to microhardness decreasing.

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Electrodeposition of [(Zn-Ni)₁/(Zn-Ni)₂]_n multilayer coatings from pyrophosphate-citrate electrolyte

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Multilayer coatings consisting of alternating nanoscale films of various compositions are promising as materials that can significantly improve protective and various functional properties of the surface of product.

Electrodeposition of multilayer $[(Zn-Ni)_1/(Zn-Ni)_2]_n$ coatings from polyligand pyrophosphate-citrate electrolyte is proposed and tested. These coatings have improved corrosion and mechanical resistance not only in comparison with zinc coatings, but also in comparison with Zn-Ni alloy coatings. It is due to creation of interlayer boundaries enriched with intermetallics, which improve the barrier anti-corrosion and mechanical properties of coatings.

The $(Zn-Ni)_1$ alloy films are deposited in the current density range of $30...40 \text{ mA/cm}^2$ (these films have free Zn, δ - and γ -phases). The $(Zn-Ni)_2$ alloy films are deposited at the current density of $6.5...15 \text{ mA/cm}^2$. This alloy additionally contain X-ray amorphous β -phase and free Ni). Increase in the Zn-Ni alloy film thickness leads to decrease in the content of free nickel in the films deposited at the current density of 10 mA/cm^2 , decrease in the content of the γ -phase. The content of δ -phase in the films deposited at the current density of 40 mA/cm^2 decreases. The content of free Zn in films of up to 100 nm thickness does not exceed 3.5%; increase in the thickness of the films by 2 leads to increase in the content of free Zn to 12-13%.

In thin layers of $[(Zn-Ni)_1/(Zn-Ni)_2]_n$ coatings the content of free Zn decreases by 2-3.8 times, the content of γ -, β -phases and free Ni occupies an intermediate position between constituent layers. Increase in number of layers leads to increase in free Zn content, and decrease in β -phase and free Ni content.

The maximum microhardness (770...865 HV) is provided by [(Zn-Ni)₁/(Zn-Ni)₂]_n coatings having the ratio the thickness of the layers h_1/h_2 in the range of 1.25...4.0 and thickness of the bilayer in the range of 40...110 nm. For comparison, microhardness of nanocrystalline single-layer coatings by γ -phase Zn-Ni alloy is only 250-500 HV.

The corrosion potentials of $[(Zn-Ni)_1/(Zn-Ni)_2]_n$ coatings in NaCl solution are naturally shifted towards more positive values with increase in nickel content in the coating up to 27-28 wt. %. They are more negative than the potential of low carbon steel in this solution. In conditions of prolonged exposure in 3.5% NaCl the $[(Zn-Ni)_1/(Zn-Ni)_2]_n$ coatings retain protective properties on steel 1.5-2.6 times longer in comparison with single-layer coatings.

Copper Ferrite as an effective photocatalyst for dye degradation under visible light

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Nowadays, environmental issues come to the fore. Particular attention should be paid to the problem of wastewater treatment from organic and inorganic contaminants resulting from the activities of the textile industry, pharmacy, chemical plants and others. Materials, capable of photocatalytic degradation of pollutants under the action of sunlight, play an important role in solving this problem [1].

Copper Ferrite nanoparticles of general formula CuFe₂O₄ were synthesized by the green method of sol-gel autocombustion. Average particles size is in the range of 20 - 35 nm, which is optimal for their use as a photocatalyst. Tauc plot was used to determine the optical bandgap (Fig. 1): $(\alpha hv)^n = hv - E_g$, where E_g

– material's optical bandgap, hv – photon energy, α – material's constant.

Small values of the optical bandgap (1.54 eV) make it possible to carry out photodegradation of contaminants under the action of visible light.





Figure 2 shows the dependence of the absorption on the wavelength at different durations of exposure to visible light. During 180 min the degree of degradation reaches a content of 98.2%.

A major advantage of such nanoparticles is the ease of removal from aqueous media due to their magnetic nature.

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Nanodimples formation on the copper foil surface after laser treatment of ZnO nanopowder

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During last years, there have been appeared different laser processing methods for the modification of various powder materials, including zinc oxide nanopowder [1]. Copper foil has long been used in experiments on laser shockwave treatment as a protective screen against direct thermal action of laser radiation.

This paper shows the nanodimples formation on the copper foil surface after laser treatment of ZnO nanopowder and explains the mechanism of their formation.

Treatment of ZnO nanopowder was performed with a neodymium laser in the Q-switched mode with a flux density of $6-9 \times 10^8$ W/cm², diameter of laser spot – 4 mm, pulse duration – 50 ns., Irradiation was carried out through a protective copper screen with a thickness of 100 µm.

Scanning electron microscopy showed that after treatment on the reverse side of the irradiated copper foil, which was in contact with the nanopowder, a large number of periodic dimples with a diameter of less than 1.5 μ m were formed. The image analysis showed that the depth of these dimples is less than 100 nm.

3 additional experiments were performed to study and explain the mechanism of formation of these nanodimples:

1) irradiation of copper foil, which was freely located on the surface of the steel substrate;

2) irradiation of copper foil on a steel substrate with liquid acoustic contact;

3) irradiation of copper foil, which is suspended on a thread (pendulum).

Analysis of experiments has shown that there are two mechanisms of nanodimples formation on the surface: the first and prevailed - caused by the stamping effect, the second - caused by the passage of a shock wave through the foil and the formation of a chipping pulse that may exceed the strength of copper.

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Dielectric function of a composite with metallic spheroidal inclusions

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The interaction of a photon with a plasmon leads to the appearance of surface plasmon-polaritons (SPP). To date, a number of plasmonic devices have been proposed on the basis of SPP. In this regard, the question arises of the influence of the geometry of metallic inclusions on the behavior of plasmon waves propagating over the surface of the composite.

Consider a composite that is a dielectric matrix with a permittivity T_m filled with identically oriented spheroidal metal inclusions. In the Maxwell-Garnett model, the diagonal components of the effective permittivity tensor of such a medium are determined by the following relation [1]:

$$\frac{\mathbf{T}_{\mathrm{eff}}^{(i)} - \mathbf{T}_{\mathrm{m}}}{\mathcal{L}_{i} \left(\mathbf{T}_{\mathrm{eff}}^{(i)} - \mathbf{T}_{\mathrm{m}}\right) + \mathbf{T}_{\mathrm{m}}} = \beta \frac{\mathbf{T}^{(i)}(\omega) - \mathbf{T}_{\mathrm{m}}}{\mathcal{L}_{i} \left(\mathbf{T}^{(i)}(\omega) - \mathbf{T}_{\mathrm{m}}\right) + \mathbf{T}_{\mathrm{m}}},\tag{1}$$

where β is a volumetric filling factor (volume fraction of inclusions); $T^{(i)}(\omega)$ is diagonal components of the dielectric tensor of the material of inclusions; \mathcal{L}_i is a geometric factor (depolarization factor), depending on the ratio of the polar *a* and equatorial *b* semi-axes of the spheroid, as well as the direction of the field ($i = \bot$, P). Factor \mathcal{L}_i takes values

$$\mathcal{L}_{\rm P} = \frac{1}{1 - \xi^2} \left(1 - \xi \frac{\arcsin\sqrt{1 - \xi^2}}{\sqrt{1 - \xi^2}} \right), \qquad \mathcal{L}_{\perp} = \frac{1}{1} \left(1 - \mathcal{L}_{\rm P} \right)$$
(2)

for fields directed along and perpendicular to the axis of rotation of the ellipsoid, respectively, where $\xi = a/b$ is the ratio of the lengths of its semi-axes. Condition $\xi < 1$ corresponds to an oblate spheroid, $\xi > 1$ corresponds to an elongated one and $\xi = 1$ to a sphere. In the latter case, $\mathcal{L}_{\perp} = \mathcal{L}_{\rm p} = 1/3$.

From formula (1), one can obtain the frequency dependence for $\tau_{eff}^{\perp(P)}$

$$\mathbf{T}_{\mathrm{eff}}^{\perp(P)} = \mathbf{T}_{\mathrm{m}} \frac{\mathbf{T}_{\mathrm{m}} + \left[\beta + (1 - \beta)\mathcal{L}_{\perp(P)}\right] \left(\mathbf{T}^{\perp(P)}(\omega) - \mathbf{T}_{\mathrm{m}}\right)}{\mathbf{T}_{\mathrm{m}} + (1 - \beta)\mathcal{L}_{\perp(P)} \left(\mathbf{T}^{\perp(P)}(\omega) - \mathbf{T}_{\mathrm{m}}\right)}.$$
(3)

In the future, expression (3) will be used to study electromagnetic waves propagating over the surface of the composite

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Layered Distribution of Structural Defects in Silicon Irradiated by Hydrogen Ions

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An ordered and controlled introduction into the crystal of the impurity or intrinsic defects and their complexes by means of the ion irradiation makes it possible to create the hidden regions with properties different from those of the matrix. The size, shape, and location of such modified regions depend on the irradiation conditions. The aim of the work was to reveal the features of the distribution of structural defects in silicon near the braking region of hydrogen ions (protons) and beyond.

To study the layered distribution of structural defects, *n*-Si samples were preliminarily irradiated at $T \le 100$ °C with 6.8 MeV protons by fluence of 10^{17} cm⁻² and annealed for 0.5 h at 580 °C. It is under these conditions that hydrogen begins to be released from Si–H bonds. Then, the samples were thinned by gradual etching from the side of irradiated surface (with a step of $30 \,\mu$ m).

Pictures of X-ray topography and selective etching of the sample taken in the irradiation plane at a depth of 315–510 µm from the irradiated surface were obtained. Taking into account that the projection path length of protons with energy of 6.8 MeV is about 360 μ m, the data are obtained for 45 μ m and 10 μ m to the braking line, as well as for 35 µm and 150 µm behind it. It was revealed that the irradiated region associated with radiation defects gradually decreases when deepening into the material, and completely disappears at a depth of about 510 µm from the irradiated surface (almost 150 µm behind the braking line). The growth layers of matrix silicon, decorated with hydrogen in the presence of oxygen, carbon and other growth impurities and defects, were found at the depth of about 395 µm (almost 35 µm behind the proton braking line). Such layers were not detected upon further etching at the depth of more than 150 µm behind the proton braking line. Micrographs of the structure of irradiated silicon after selective etching, which fix changes in the structure near the proton braking line at the corresponding depths, showed that the proton path region remains crystalline with detected typical defects, and the silicon structure changes behind the braking line.

Thus, the research results of radiation-stimulated modification of silicon defective structure have shown that collective interaction processes under conditions of high density of atomic collisions can contribute to inner phase transformations, causing the formation of defect layers and changing the matrix parameters.

Optical properties of nickel molybdate hydrate/carbon material composite

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Nowadays, nickel molybdate (NiMoO4) is a promising material for the electrodes of electrochemical capacitors, due to its structural, electronic and electrochemical properties. The formation of composites based on it with carbon material allows to increase the specific surface area and, accordingly, increase the kinetics of ion transport. The hydrate NiMoO₄ / C composite was obtained by the hydrothermal method [1]. Raman spectroscopy was used to study the optical properties of the composite.

The registered relatively intense bands with maxima of 947, 870, 828 and 354 cm⁻¹ [2] are characteristic for NiMoO₄, in which Ni²⁺ cations have octahedral coordination, while Mo⁶⁺ ions are in tetrahedral coordination. We also registered a band of low intensity at 1050 cm⁻¹, which is probably due to fluctuations of bending modes of coordinated water. In the Raman spectrum of the composite, bands in the range of 1100-1750 cm⁻¹ are additionally registered. To characterize the carbon material in the synthesized composite, the experimental Raman spectrum in this range was decomposed into five components: D, D', D₃, D₄ and G bands. The G-band (1580-1590 cm⁻¹) corresponds to the fluctuations associated with the doubly degenerate E_{2g} mode of the center of the Brillouin zone and is the result of the fluctuation modes of all pairs of carbon atoms with sp²-hybridization forming benzene rings. The Dband is the result of the manifestation of a breathable A_{1g} mode, which is activated by defects at the K point of the Brillouin zone and is observed only in the Raman spectra of defective carbon samples. For the same reason, the presence of defects is also a prerequisite for the observation of the band D' (1620 cm^{-1}). As for the band D_3 , it is due to the contribution of scattering of the amorphous phase. Finally, the D₄ band is manifested in the spectra of carbon materials containing polyenes and ionic impurities [2].

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Electrochemical properties of NiMoO₄ / carbon material composite

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At present times a great deal of attention is being paid to multifunctional nanocrystal materials, namely nickel molybdates and composites with carbon material based on them [1]. The electrochemical behavior of the NiMoO₄ / C composite in the 6 M KOH electrolyte was investigated by cyclic voltammetry and galvanostatic charge / discharge testing.

Redox peaks of the composite (Fig. 1 a) are the result of the interaction of Ni²⁺ ions from the structure of molybdate with OH⁻ groups from the electrolyte, followed by the formation of $Ni(OH)_2$. During the charge, oxidation of nickel hydroxide to nickel oxyhydroxide takes place. During the discharge, nickel ions are reduced. It should also be noted that along with the intercalation of protons in the crystal structure of Ni(OH)₂, K⁺ ions are intercalated from the electrolyte into the of NiOOH, layered structure which explains the asymmetry of the redox peaks of the materials. The nonlinear shape of the discharge curves (Fig. 1 b) confirms the Faraday type of charge accumulation due to the intercalation of electrolyte ions in the structure of the material and redox reactions, and agrees well with the available peaks cvclic on the voltammograms of the composite. Carbon material with a large number of micro- and mesopores is an ideal matrix for the



Fig. 1. The cyclic voltammograms and discharge curves of NiMoO₄/C composite.

deposition of nanocrystal NiMoO₄, avoids agglomeration of nanoparticles and at the same time forms an interconnected conductive network.

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CdTe-PbTe superlattices with quantum dots

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The formation of CdTe-PbTe quantum dots (QDs) was performed by a specially developed infrared laser epitaxy technology with *in situ* growth and temperature control, which allows to significantly reduce the growth temperature ($\Delta T \sim 200$ K) and carry out the entire process in one cycle. The structures were grown using two types of substrates - (111) CdTe and glass covered with a transparent in the visible region and with a high conductivity (8 Ohm / \Box) InSnO2 layer (ITO). The buffer layer was not grown. The number of layers of each of the components in both cases was the same and was equal to 50, the thickness of the layers was 10 nm. Analysis of AFM results showed the presence of densely packed QDs with some difference in size, from 4 to 20 nm on CdTe substrates and a much smaller scatter on ITO - 4-10 nm. Given the parameters of bulk crystals, the pair of PbTe-CdTe semiconductors, as well as PbS-CdTe and PbSe-CdTe belong to the I-type structures, but in the transition to



Fig.1. PL CdTe-PbTe SLQD on CdTe substrate (1) and on ITO substrate (2).

the quantum architecture, as established experimentally and from calculations of the band structure of superlattices with quantum dots (SLQD), passes to the II-type structures, with a radius of PbTe QDs $r \le 6$ nm. The electronic structure of SLOD determined from is studies low-temperature of photoluminescence (LTPL) at T = 5K in a wide spectral range, including the visible region (1-2.5 eV). As a result of LTPL studies, it was found that the edge region of LTPL

SLQD (Fig. 1) is significantly shifted to the high-energy region relative to the source material from which the CdTe film was grown on InSb substrates under the same technological conditions as SLQD.

QDs of both components of SLQD have a perfect crystal structure, as evidenced by the presence in the LTPL spectrum, in addition to purely electronic transitions, a series of peaks corresponding to the emission of longitudinal optical (LO) phonons for CdTe ($hv_{LO} = 0.019eB$)

Influence of the concentration of adsorbed atoms on the height of surface irregularities of semiconductors with the Zinc blende structure

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The creation of a new class of sensitive sensors, heterolasers, filters and other modern opto- and nanoelectronic devices with controlled parameters requires the study of the mechanisms of electronic states excitation on the adsorbed surface and mechanisms of scattering of charge carriers on the semiconductor surface. One such mechanism is the dynamic deformation in the subsurface solid layer, which can be created by the quasi-Rayleigh acoustic wave and adsorbed atoms. Depending on the adatoms concentration, the nonlocal elastic interaction of adatoms with a self-consistent quasi-Rayleigh wave through the deformation field affects the shape and height of the semiconductors surface irregularities created by the dynamic deformation field.

Therefore, there is a need for the theoretical study of the effect of the change of adatoms concentration, of the interaction of adsorbed atoms with each other and with the surface acoustic wave on the surface characteristics, in particular the effect on the height of semiconductor surface irregularities and the deformation potential of quasi-Rayleigh wave.

The mathematical model of this problem was built on the mechanism of deformation interaction created by a quasi-Rayleigh wave and adsorbed atoms, which is described by a self-consistent system of nonlinear differential equations: mechanical equilibrium equation; the diffusion equation renormalized by the acoustoelectronic effects; Poisson's equation taking into account the redistribution of electric charge under the action of deformation; continuity equation for electric charge; electroneutrality conditions with self-consistent boundary conditions.

Within the model of nonlocal elastic interaction of adatoms with a selfconsistent acoustic quasi-Rayleigh wave through the deformation field, the height of surface irregularities on the adsorbed surface of monocrystal with the Zinc blende structure depending on the concentration of adsorbed atoms was calculated. It was established that the functional dependences of the height of surface roughness and deformation potential on the adatoms concentration have a nonmonotonic character due to two competing factors: mechanical deformation of the surface crystal lattice created by mechanical action of adatoms (geometric scale factor), and interaction of adatoms through a deformation field created by a surface acoustic quasi-Rayleigh wave and adsorbed atoms.

Spectral properties of open multi-cascade nanostructure as an element of quantum cascade detector

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Production of quantum cascade lasers (QCL) and quantum cascade detectors (QCD) operating in infrared range is stimulating the development of the theory of physical processes in multi-layered nanostructures, which are the basic functioning elements of these nano devices. It is well known [1, 2] that the main structural element of typical QCD and QCL consists of the same multi-layered nanostructures – cascades. Therefore, in the majority of theoretical papers a simplified model of separate cascade was studied because the properties of all cascades were assumed as the same. However, according to the principles of quantum mechanics, it is evident that the properties of the system, which consists of many interacting subsystems – cascades should be essentially different from that of single-cascade structure.



Fig.1. Potential profile of open nanostructure, being a main element of multicascade QCD

In the proposed paper, within the model of rectangular potentials and position-dependent effective mass of electron and using the exact solutions of Schrodinger equation, the transmitting coefficient is calculated for the multicascade open nanostructure (fig.1), which is the model of the main element of typical QCD operating in far infrared range. This transmitting coefficient made it possible to study the properties of resonance energies and resonance widths of electron quasi-stationary states in multi-cascade model.

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The temperature effects in plasmonics of the metallic lowdimensional structures

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The temperature dependence of the spectral characteristics (the frequency of the surface plasmonic resonance, the relaxation rate of electrons) of the metallic nanoparticles plays the significant role in their practical use (thermomagnetic information recording, catalysis and synthesis of the nanostructures, the production of the different chips, the thermal destruction of the malignant tumors). Accordingly, the study of the temperature effects on the plasmonic phenomena in the metallic nanoparticles is the actual problem.

As the temperature rises, the shift of the frequency and the broadening of the surface plasmonic resonance line take place. The physical mechanisms, which lead to this, are the thermal expansion of the nanoparticles and the increase of the rate of the volume relaxation due to the enhancement of the role of electron-electron and electron-photon scattering.

The decrease of the concentration of free electrons and, hence, the decrease of the frequency of the bulk and surface plasmons take place under the thermal expansion of the nanoparticles. Such decrease of the frequency of SPR leads to the red shift of the absorption peak. The temperature dependences of electron-electron and electron-photon relaxation rates have the form:

$$\gamma_{\text{e-e}}(T) = \gamma_{\text{e-e}}(T_0) \left[1 + \left(\frac{h\omega}{2\pi k_{\text{B}}T}\right)^2 \right], \qquad \gamma_{\text{e-ph}}(T) = K'T^5 \int_0^{\Theta_{\text{D}}/T_0} \frac{z^4 dz}{e^z - 1},$$

where

$$K' = \gamma_{\text{e-ph}} \left(T_0 \right) \left\{ T_0^5 \int_0^{\Theta_{\text{D}}/T_0} \frac{z^4 dz}{e^z - 1} \right\}^{-1}$$

and $\Theta_{\rm D}$ and $z = f(\Theta_{\rm D}/T)$ – Dubye temperature and Dubye function; $\gamma_{\rm e-e}(T_0)$ and $\gamma_{\rm e-ph}(T_0)$ – electron-electron and electron-photon relaxation rates at some fixed temperature T_0 .

By this means, the increase of electron-photon relaxation rate under the increase of the temperature results in the broadening of the absorption peak.

The results of the performed calculations show that the decrease of the frequency of SPR due to the thermal expansion and the increase of the bulk relaxation rate, in turn, result in the decrease of the absorption by the metallic nanoparticle under the rise of its temperature.

Generation of A^{II}_{1-x}TM_xB^{VI} (TM: Mn, Co, Cr) nanostructures by pulsed laser ablation in liquid

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During last decades, generation of semiconductor nanoparticles under laser ablation of solid target in gas or in vacuum has been extensively explored. The process of pulsed laser deposition (PLD) was widely used for a large variety semiconductor compounds including so-called diluted magnetic of semiconductors (DMS). This is comparatively new class of materials with unique properties caused by spin exchange interactions between magnetic ions and band carriers (electrons and holes). On the other hand, formation of semiconductor nanostructures under pulsed laser ablation in liquid (PLAL) is less studied, although this technique has many advantages compared to other growth routes. The mechanisms of laser induced thermal vaporization and phase explosion are still far from understood and they are highly dependent on the inhomogeneous energy deposition in different atmosphere (air or liquid condition).

In the present work, we report on experimental investigations of structural and optical properties of CdTe- and ZnO-based DMS, which are in form of micro- and nanoparticles generated by PLAL technique.

Micro- and nanostructures were produces by pulsed laser ablation of target in deionized water. The target was irradiated using Nd:YAG pulse laser (1064 nm) operating at 10 Hz with pulse width of 10 ns and power of 1 W. Ceramic plates of ternary $A^{II}_{1-x}TM_xB^{VI}$ (TM: Mn, Co, Cr) solid solutions as targets were applied. The laser beam was focused on the target with a 1.5 mm spot by a quartz lens with 120 focal length. After laser ablation the colloidal solution or the dropped layer onto Al substrate were the samples for investigation.

X-ray diffraction (XRD), scanning electron microscopy (SEM) and atomic force microscopy (AFM) techniques were used for structural and morphological analysis of the fabricated nanostructures. The high-resoluion SEM microscopy clearly illustrates flower-like particles of ZnO-based DMS, which consist of nanosheets and nanoleaves with average thickness about (5-8) nm. Obviously, these nanoobjects are responsible for the observed blue shift of the absorption edge in DMS nanostructures. In magneto-optical Faraday rotation spectra of all samples there were exhibited peculiarities associated with s,p-d spin exchange interactions and confinement effect. The observed main features were compared also with those obtained for related nanoparticles prepared by methods of colloidal chemistry.

Renormalized spectrum of localized quasiparticles interacting with single- and two-mode phonons at T≠0 K in Davydov's model

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Intensive use of multilayered nanoheterostructures, being the basic structure elements of successfully functioning nanodevices (quantum cascade lasers and detectors operating in infrared range) is permanently stimulating the development of the theory of quasiparticles (electrons, excitons, impurities) interacting with multi-mode phonons (confined, interface, propagating and so on).

Due to the known mathematical problems in quantum field theory, a consistent theory of renormalized spectra of multi-band (even one-band) systems of quasiparticles interacting with multi-mode phonons is absent till now. In the well known Davydov's work [1], the simplified model of the system was studied. It described the localized quasiparticle (in two possible states) interacting with multi-mode non-dispersive phonons. The method used for the unitary transformation of operators, made it possible to perform the exact calculation of two-time retarded Green's function at $T \neq 0K$ in general analytical form. However, the Fourier-image of this function and, since, the renormalized spectrum) was exactly obtained only for the single-mode system. The renormalized spectra for the two- and multi-mode systems were calculated within approximation, which was valid only at the condition of high temperature of the system.

In the proposed paper, using the Hamiltonian for the two-mode Davydov's model, which describes the interaction between the localized quasiparticle and non-dispersive single- and two-mode phonons at arbitrary temperature, we, for the first time, exactly analytically calculated the Fourierimage of quasiparticle's Green's function. As the result, the exact analytical expressions are obtained for the renormalized energy spectrum and average numbers of phonons in quasiparticle "dresses" for the main and all satellite states.

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Quinoid structure of oxidized oligomers of 3,4-ethylenedioxythiophene

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An investigation of a CP is mainly reduced to clarifying the nature and properties of their charge carriers that usually consist of polarons or/and bipolarons with or without spin. Studies of this kind can crucially facilitate the development of new CP-based materials with improved properties for their subsequent application in molecular electronics.

The most extensively studied CPs are polythiophenes, in particular, poly(3,4-ethylenedioxythiopehene). However, even the latter lacks a reliable information on the nature of its charge carriers and their dependence on the polymer-chain length.

In this work we apply the Kohn-Sham density functional theory (B3LYP / $6-31G^{**}$) to study the electronic and spatial structure of the 3,4-ethylenedioxythiopehene oligomer consisting of its 12 units (E12), in its various charge states: 0, +1, +2, +3, and +4.

Calculated C-C bond length between neighboring monomeric units amounts 1.433 Å for the electroneutral state of E12 that is typical for a benzenoid phase. However, even an insignificant extent of doping (being simulated by the cation $E12^{+1}$) leads to a monotonous shortening those bonds from the ends of the chain to its center with the minimal value of 1.417 Å at bond 6; the latter being typical for a quinoid structure. The dication $E12^{+2}$ shows similar behavior of the abovementioned bond lengths. However, the latter are noticeably smaller in comparison with the similar bond lengths in $E12^{+1}$, thus showing an increase of the quinoid-phase contribution. Higher oxidation states (+3 and +4) show two minima near bonds 2 and 3, as well as 9 and 10 that evidences in favor of a further increase of the quinoid-phase contribution as well as a formation of two separated polarons at the ends of the oligomer chain.

The HOMO-LUMO gap in the neutral E12 amounts 2.06 eV. As the positive charge (as a model for an increasing doping extent) grows, we observe a progressive appearance of one $(E12^{+1})$, two $(E12^{+2})$, three $(E12^{+3})$, and four $(E12^{+4})$ polaron levels within the abovementioned HOMO-LUMO gap. A single polaron level in $E12^{+1}$ is separated from the top of the valence band by 0.54 eV.

Thus, according to our model, the conductivity of a highly doped (oxidized) 3,4-ethylenedioxythiopehene oligomer consisting of its 12 units is provided by two polarons situated at the ends of the chain. For other oligomers, as well as for poly(3,4-ethylenedioxythiopehene), more sophisticated polaron structures might act as charge carriers.

Synthesis of «porous silicon – cadmium telluride» nanocomposites and study of their properties

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Currently, there is great interest in composite systems, which consist of a matrix and embedded in the matrix of materials or nanoobjects. The interest is due to the fact that the control of the physical properties of such systems can be carried out in a wide range by modifying both the matrix itself and the material embedded in it, for example, technological methods. The creation of composite structures based on matrix and nanocrystals (NC) of a semiconductor is very important. Composite structures can be created by introducing into the matrix of colloidal solutions of NC with subsequent processing at a certain temperature.

We have developed an original method of colloidal synthesis of monodisperse NC CdTe with high stability, narrow bands of photoluminescence (PL) and high quantum yield. A composite system based on porous silicon (PS), which serves as a matrix, and NC CdTe, which are incorporated into the porous matrix, were obtained. The peculiarity of this system is that both components have PL of different intensities. The large difference in PL intensities and different positions of the radiation bands allowed, comparing the PL spectra of the colloidal solution of NC CdTe, PS and NC CdTe – PS at different stages of introduction of CdTe nanoparticles into the porous silicon surface, to identify the interaction and mutual influence of the two constituent materials.

The colloidal solution of NC CdTe was applied to the surface of the PS sequentially by spraying, drip method and the method of precipitation of particles from a fixed volume and subsequent evaporation at a temperature below 100°C. In order to intensify the process of precipitation of CdTe particles in the solution was introduced isopropyl alcohol, which is a solvent with a low coefficient of sedimentation stability in a number of solvents for this system. The dependence of PL intensity on the density of CdTe particles deposited on the PS surface was measured and the PL spectra of the PS – NC CdTe system were recorded at different stages of CdTe nanoparticle deposition on the porous Si surface.

The introduction of NC CdTe into the porous surface creates a strong stable structure. The planned change of properties of PS and colloidal solutions of NC CdTe by variation of technological methods of synthesis and processing methods will allow to control the physical properties of this composite system in a wide range and to use new principles of design and creation of new generation sensor devices.

Ion beam-induced surface topology of two-component materials with near-non-preferential sputtering

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Ion sputtering is one of the relatively simple methods for fabrication of surfaces covered with cone arrays having a significant potential for practical application, in particular, for development of field-emission devices. Here we discusse the peculiarities of the formation of ion-induced surface topology of two-component materials under conditions of sputtering close to non-preferential. Usually sputtering of multicomponent materials is preferential, due to differences in the atomic masses of the constituents and their surface binding energies. However, with a certain combination of these parameters the sputtering of the multicomponent materials may be close to non-preferential. Such a situation, as we have recently shown [1], occurs in SnTe crystals, which creates good preconditions for the study of this issue. Investigating the sputtering of SnTe crystals by argon ions of different energies, for the first time we experimentally observed formation of dense cone arrays on a sputtered surface as a result of near-non-preferential sputtering of multicomponent compound [2].

The main feature of SnTe sputtered surfaces topology is a dense undergrowth of small surface structures having the shape of ordinary cones. The height of such cones is limited by the size of the nanometer range. This undergrowth fills the space between dispersed "high" (micrometer range) conical structures having the shape of ordinary or truncated cones. The apex angle of the highest generation ordinary cones and the angle between generatrixes of the truncated cone very closely coincide. Dispersed arrays of high cones are apparently formed by a well-known mechanism of ion collisions with the surface, when the growth of conical structures is initiated by the presence of protective masks covering the top of the cones. The details of the undergrowth cone formation mechanism are not yet fully understood. We suggest that the cone undergrowth formation is initiated through formation of nuclei of a new phase on the sputtering surface as a result of re-deposition of the sputtered species. All these issues are analyzed in detail and discussed in the presented report.

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ORAL REPORTS

Session 3 Physical-chemical properties of thin films



Size effect in the composite thin film of Bi - Pb alloy

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Nanofilms and dispersed metal compounds are promising objects of research for nuclear energy, as they are able to function stably for a long time in cyclical external fields of temperature, pressure and radiation. Bi-Pb system is one of the promising materials for practical use in new reactors with heavy liquid metal coolant [1]. Hereby the problem of phase stability is relevant for such materials and thin films.

In our investigation we elaborate a new theoretical approach based on the size-dependence of the atomic cohesive energy [2-3]. It allows constructing different size-dependent thermodynamic models and the drawing of phase maps [4]. We apply the new methodology in the framework of regular (subregular) solution model for the thermodynamics and phase stability of thin film of Bi - Pb alloy (fig.1).



Fig.1. Fragment of the phase map of a continuous Bi-Pb nanofilm

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Structure and barrier characteristics of modified polyethylene films

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Modified polymeric film materials are used as the most accessible and cheapest type of metal and electronic devices protecting and packaging. Low density polyethylene (LDPE, up to 67 wt. %) was chosen as the basis for the studies. Mineral material such as Credolen (up to 25 wt. %) was as filler used. Gas corrosion inhibitors and plasticizers were as additives. For instance an inhibitor (from 1,0 wt. % contain) used dicyclohexylamine benzoate (DCHAB), as a plasticizer – dibutyl phthalate (DBP). The plasticizer was injected into polymer matrix for facilitation processing and for combining with matrix material. The film thickness was near $120\pm5 \,\mu\text{m}$.

Oxygen permeability of polyethylene film material was determined by manometric method.

It was found that fillers significantly reduce the initial oxygen permeability of materials (P = $3 \cdot 10^{17} \frac{m^3 \cdot m}{m^2 \cdot s \cdot Pa}$). However, during operation for 5 years of such material there is an increase in the value of oxygen permeability (P = $7.5 \cdot 10^{17} \frac{m^3 \cdot m}{m^2 \cdot s \cdot Pa}$), which indicates an increase in the activity of destructive processes over a short period. Additions of plasticizer significantly slow down the processes of destruction of the matrix and keep for a time oxygen long the permeability index at the level $(P = 4-4, 5 \cdot 10^{17} \frac{m^3 \cdot m}{m^2 \cdot s \cdot Pa})$. In films with inhibitor additives, there is a significant increase in gas permeability and a decrease in the protective and

significant increase in gas permeability and a decrease in the protective and barrier function of the film during the second year of operation. Increase of film thickness up to $160\pm5 \mu m$ leads to decreasing of diffusion transfer through the material by 1.1-1.2 times.

Co-injection of gas corrosion inhibitors with mineral filler initially increased the corrosion protection of metal products in the package, but at the same time increased the crystallinity of the polymer matrix and reduced the intensity of diffusion oxygen transfer through the film. However, during long periods of storage in such films, destructive processes are activated, leading to the formation of through pores and the destruction of the integrity of the coating.

Simultaneous injection mineral filler and inhibitor into the composition of the polymer matrix stabilized the diffusion processes in the material during the whole service life.

The features of optical absorption and structure of poly-ortho-anisidine think films doped with graphene oxide

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A great attention now attracts the conjugated polymers with intrinsic electron conductivity such as polyaniline and their derivatives. The electrooptical properties of polyaminoarenescan be changed by doping with electronic donors or acceptors that generate n- and p-type charge carriers [1]. We studied the effect of graphene oxide (GO) on the structure and optical absorption in the visible and near IR regions of poly-ortho-anisidine (PoA) think films. Polymer films on transparent SnO₂ substrates were prepared by the method of electrochemical polymerization in the mode of cyclic voltammetry.

The absorption spectra of poly-ortho-anisidine films are characterized by three bands. The band with energy maximum E = 3.25 - 3 eV is due to the π - π * transition in the band gap. The second band at E = 2.1 - 2 eV is associated with the $n \rightarrow p$ transition in the benzoquinoid system, and the absorption with a maximum of E = 1.7 eV corresponds to delocalized charge carriers. As a result of doping the PoA film with graphene oxide, the absorption in the long-wavelength region of the spectrum decreases is observed. The optical band gap in result of doping of PoA film with GO decreased from 1.21 eV to 1.14 eV due perhaps to increasing of the number of charge carriers.

According to transmission electron microscopy (TEM) data, the PoA film is characterized by an amorphous structure with structural element sizes of 20–30 nm. Doping the film with GO changes the morphology of the nanolayer with the formation of individual sections of graphene sheets, and the size of the structural elements increases to 200–300 nm.

Doping with PoA with graphene oxide causes a change in the optical absorption and structure of the polymer film. It can be assumed that the interaction of GO with the polymer reduces the energy of the electronic transition of charge carriers due to the ordering of the structure in the composite nanolayer PoA-GO.

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XRD and **ND** study and structural changes in Ge-S-Ag glasses

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Nowadays are increasing amount of digital information, and the demand on memory devices being able to store, communicate, and compute this information is also increasing. Currently, flash memory based on charge storage is widely used in cell phones and music players and continuously replace hard disc drives in PCs and even in data centers. However, flash memory is challenged by a down-scaling problem because of the charge leakage from the storage layer. In this view, alternative memory technologies such as, for example, phase-change memory (PCM) and conductive-bridge memory (CBM) have been suggested.

Work of PCM is based on a non-volatile reversible switching of an active material, e.g. Ge-Sb-Te chalcogenide, from amorphous to crystalline state characterized by remarkably different electrical resistivity. The amorphous-to-crystalline transformation is thermally controlled by the current passing through the material.

It has been known for a long time that chalcogenide glasses (ChG), which are basically semiconductors, become superionic conductors upon doping with metal species. Ge-S-Ag glasses are very attractive, first of all, due to significantly higher glass transition temperature and consequently better thermal stability compared to the other based glasses. Also, Ge-S-Ag glasses are free of toxic elements.

In this work, we perform a microstructural study of GeS_2 -Ag, $Ge_{42}S_{58}$ -Ag and GeS_3 -Ag chalcogenide glasses, extending the accessed composition range. Investigations along ChG-Ag lines are also of interest in a view of the CBM applications, in which a chalcogenide glass acts as a matrix and Ag atoms diffuse into the matrix from a silver electrode.

We have been analized the maxima of the intensity of the main three XRD and ND peaks and compared with the corresponding SEM images. The intensity of the XRD first sharp diffraction peak (FSDP) of $(GeS_3)_{100-x}Ag_x$ and $(Ge_{42}S_{58})_{100-x}Ag_x$ glasses decreases, while its position at about 1.06 Å⁻¹ remains constant.

The second maximum shifts to smaller values of the diffraction vector Q and its intensity increases. The next maxima also shift to lower Q-values but the intensity of oscillations decreases with increasing Ag concentration.

The more detailed analysis reveals that for homogeneous $(Ge_{42}S_{58})_{100-x}Ag_x$ glasses position Q_{FSDP} increases practically linearly, whereas that for the phase separated glasses $(GeS_3)_{100-x}Ag_x$ and $(GeS_2)_{100-x}Ag_x$ deviates from the linearity.

The effect of interband 3d-4s transitions in Cu on the Kerr ellipticity in the multilayer synthetic antiferromagnet Co/Cu prepared by magnetron sputtering

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In this report we present the results of the Kerr ellipticity study in the $Co(0.9nm)/Cu(1.8nm)_{20}$ multilayer produced by the magnetron sputtering method. Previous measurements of Co/Cu(111) multilayers with different thickness of Cu layers, carried out for light with $\lambda = 632.8$ nm, showed an increase in the Kerr rotation of the films, where the thickness of the Cu layers ensured the antiferromagnetic (AFM) bonds between the ferromagnetic (FM) Co layers. It has been suggested that the increase in the Kerr effect is caused by the hybridization of electron states in the Co/Cu interfaces and by increased number of the Co-clusters created during formation of the cobalt layers under conditions of the electronic size quantization in the Cu layers. Here the Kerr ellipticity were measured at different wavelengths of light. The dependences of ellipticity on the magnetic field $\eta(H)$ are shown in Fig.1. The linear increase of $\eta(H < 1 \text{kOe})$ corresponds to the gradual alignment along H of magnetic moments of the FM Co-layers in the spin-flop phase of the AFM ordered regions of the multilayer. The further increasing of η at H>3kOe is determined mainly by magnetization of the Co-cluster. These parts of the dependences $\eta = \eta_{\rm FM} + \eta_{\rm SPM}$ are different for light with different light wavelengths. The largest increase in ellipticity is observed for 600 nm (Fig. 2). The revealed feature indicates that the enhancement of the magneto-optical Kerr effect in the Co/Cu(111) multilayers is connected with influence of interband 3d-4s transitions in the hybridized electronic system of Cu having gap between bands equal to 2.1 eV.



Fig.1 and Fig.2 The magneto-field dependences of the Kerr ellipticity of the longitudinal Kerr effect obtained for $\lambda = 500$ and 600 nm (1) and ratio of the Kerr ellipticities caused by superparamagnetic cluster and FM subsystems in the multilayer [Co(0.8 nm)/Cu(1.8 nm)]₂₀ (2).

Photoinduced changes of the optical properties of (Ga_{0.3}In_{0.7})₂Se₃ films

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 $(Ga_xIn_{1-x})_2Se_3$ mixed crystals with the concentrations 0.02 < x < 0.55 belong to a defect wurtzite structure with hexagonal symmetry (space group *P*61 or *P*65). The main feature of these semiconductors is high concentration of the vacancies which can form spirals along the optic axis *c* of crystal. Recently a number of studies of $(Ga_xIn_{1-x})_2Se_3$ films have been performed, with the emphasis at their efficient applications.

In this paper, we report on the optical studies of $(Ga_{0.3}In_{0.7})_2Se_3$ films irradiated with a green laser. In addition, we analyze the effect of laser irradiation on their optical transmission spectra, parameters of the Urbach absorption edge, and refractive indices.

We have shown that the optical absorption edge for non-irradiated and irradiated $(Ga_{0.3}In_{0.7})_2Se_3$ films has an exponential shape. The influence of irradiation on the optical parameters of the films under study is analyzed.



Fig. 1. Dependences of the energy pseudogap E_g^{α} (1), Tauc energy E_g^{fauc} (2) and Urbach energy E_U (2) on the irradiation time for $(\text{Ga}_{0.3}\text{In}_{0.7})_2\text{Se}_3$ films.

The largest changes in the optical parameters during irradiation are observed in the first 2 minutes, then with increasing exposure time the level of photoinduced changes decreases. Thus, with irradiation time increase the energy pseudogap increases and the Urbach energy decreases. The behavior of the refractive index is more complicated. During the first minute of irradiation, the refractive index decreases and then increases.

Influence of surface morphology on electrophysical properties of PbTe: Bi films

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The hypothesis of correlation of morphological and electrophysical properties of PbTe: Bi films of different thickness deposited on sitall and mica is tested in the work.

Semiconductor structures based on PbTe films are often used in the creation of detectors and radiation sources of the infrared region of the optical spectrum and thermoelectric energy converters. Interest in such structures is associated with the study of dimensional and quantum effects [1].

Polycrystalline films were precipitated from the vapor phase by open evaporation in a vacuum of PbTe: Bi 1 at.% on fresh chips (0001) of mica and purified sitall. The temperature of the evaporator was $T_V = 700$ °C, and the temperature of the substrates during the deposition of $T_S = (150-200)$ °C [2].



Fig. 1. The thickness dependence of the shape parameter of surface objects k, which characterizes the ratio of height to diameter, and the mobility of charge carriers for films grown on sitall.

The thermoelectric characteristics of PbTe: Bi thin films on sitall substrates (Fig. 1) are considered and their relationship with the morphological characteristics of the film surface is revealed. A similar situation is for films grown on mica.

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β-CdTe based heterostructures

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Cadmium telluride is one of the important materials of modern electronic technology. Its physical and technical parameters determine the possibility of using it in solar energy devices. However, the crystals β -CdTe serve as the basic material for the manufacture of various devices of functional electronics, for which an important issue is the extension of the spectral range of photosensitive and light-emitting devices to the short-wavelength blue-violet region.

 β -CdTe / CdS / ZnS heterostructures based on cadmium telluride crystals have been obtained. Their production was carried out using the isovalent substitution method. For this, carefully prepared substrates of CdTe crystals of the cubic modification were placed in evacuated quartz ampoules with corresponding weighed portions. They provided the possibility of sequential isovalent substitution. Heterospheres β -CdS and β -ZnS were formed due to the diffusion of the corresponding elements along the anionic and cationic sublattices in accordance with the reactions

> β -CdTe + S $\rightarrow \beta$ -CdS + Te β -CdS + Zn $\rightarrow \beta$ -ZnS + Cd

The production of new materials is confirmed by complex studies of optical reflection, absorption and luminescence using modulation spectroscopy (λ -modulation). The high sensitivity and accuracy of the technique made it possible to unambiguously determine the characteristics and properties of heterostructures and for the first time determine the parameters of the energy structure of CdS of an atypical cubic modification, namely, the band gap Eg = 2.90 eV and the spin-orbit splitting $\Delta_{SO} = 0.30$ eV. For β -ZnS layers, the parameters of the energy structure agree with the known ones -Eg = 3.68 eV, $\Delta_{SO} = 0.072$ eV. The high structural perfection of the components of the β -CdTe / CdS / ZnS heterostructure is confirmed by the effective photoluminescence in the edge region. The emission spectrum covers the range of photon energies $\hbar\omega = 2,30 - 3,85$ eV with the corresponding maxima of the components in the region of 2,71 eV, 2,85 eV and 3,62 eV for the heterostructure material. The mechanism of the formation of radiative recombination is discussed.

Dispersion kinetics of thin double niobium-copper films deposited onto oxide ceramic materials and annealed in vacuum

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In modern technology there is a need for the production of permanent vacuum-tight precision ceramic joints with an ultra-thin seam. Such joints can be made by brazing or pressure welding of metallized ceramic parts. This purpose can be achieved by application onto ceramic surfaces of double metal films, one part of which is 100 - 200 nm thickness and consists of an adhesion-active metal (e.g. Ti, Cr, Nb, Ni etc.), and the other layer is slightly thicker (1 – 3 microns) and serves as a solder (e.g. Cu, Ag etc.) ensuring joining of metallized ceramic materials during brazing or pressure welding with a fine brazed seam (2 – 4 microns thickness).

In this work, specimens were used made of alumina and dioxidezirconium ceramics and metallized with a 150 nm niobium nanofilm and then atop, by a 1,5 – micron copper film serving as a soldering metal for ceramic samples joining. Copper was chosen as a solder in view of the fact that it is able to wet niobium well, and also it does not interact with niobium forming new phases.

The study found that, the first slight changes in integrity of the original niobium-copper films onto oxide materials appeared only after 20 min at this temperature. The situation did not change virtually with increase of the annealing temperature up to 1000°C, at which noticeable changes in the films morphology were found also after 20 min of exposition. Raising the annealing temperature up to 1050°C intensified the process of changing the films morphology, which was noticeable already after 10 min of exposition. After 20 min of annealing, there was a noticeable tendency for the dispersion in the films, although they were still covering even more than 80% of the substrate surface. Significant dispersion of the films was caused only by annealing at 1100°C, when the copper had to be already in molten state, which is clearly visible after 5 min of exposition. After 10 min of exposition, and especially after 20 min of annealing, the films were strongly dispersed, although their residues were still covering more than 70% of the substrates surface area.

According to the results of the studies, kinetic decay curves of the investigated thin double metal films were constructed, by which the basic technological parameters of the processes of joining ceramic materials by soldering or welding using data prototypes of data connections were made ceramic with a soldering gap of $2 \div 3$ mcm. The shear strength of the obtained ceramic joints was ~ 150 MPa.

Influence of UV radiation and atmospheric factors on vapor permeability of thin-film modified polyethylene materials

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The leading factors of action on electronic devices and metal products during storage in polymer packaging are different types of gases, as well as vapors of various organic compounds and water vapor. Contact of a small amount of the above substances - agents of influence on the defect-free operation of devices, leads to the activation of oxidation processes on metal components, damage and blockage of conductive paths, changes in the electronic structure of materials etc.

The researches of films vapor permeability were performed by weight method (dry cup method), using metal cups, according to international documents ISO 7783, ISO 2528 and ASTM D 1653.



The initial vapor permeability of unmodified polymer films, defined as the "water vapor transfer rate", was set at a level WVTR = 0.12-0.13 $\frac{mg}{m^2 \cdot s}$ (after 30 days of stabilization). Films modified with atmospheric corrosion inhibitors, plasticizers and Al additives had an initial vapor permeability, usually lower. WVTR = 0.09-0.13 $\frac{mg}{m^2 \cdot s}$.

The vapor permeability coefficient of UV irradiated films may differ due to changes in the intensity of structural processes as under the internal influence (composition type and

structural processes as under the internal influence (composition, type and quantity of additives) and external (intensity and time of radiation, outdoor exposure so on) factors. UV irradiation for 200 hours inevitably led to a slight increase in vapor permeability (Fig.).

However, if the WVTR coefficient increased by 46% for unmodified samples, then for modified ones - on average by 9-16% depending on the content of modifying components (except for films with DBP plasticizer).

Small concentrations of additives significantly affect the change of structure, which is especially evident during long-term operation (more than 4 years) of coatings in open areas.

Influence of B₂O₃ additives on optical and operational properties of the ZnS-Ge system and the resulting thin-film coatings

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Zinc sulphide and elemental germanium are one of the most important materials for infrared optics - both for the manufacture of substrates and for the deposition of interference coatings. Recently, a ZnS-Ge composite has been proposed as an independent material for obtaining coatings with a high (about 3.0) refractive index.

Its evaporation and condensation in high vacuum, most likely, occurs by the CVD (Chemical Vapor Deposition) – mechanism. Upon condensation, a nano-dispersed coating is formed on the substrate, which has a very high mechanical durability.

However, the insufficient reproducibility of the coating parameters, due primarily to the presence of oxide impurities (ZnO, GeO₂) in the composite, prevents the widespread use of the material. The use of a B_2O_3 additive, which plays the role of a composition stabilizer due to the binding of oxide impurities into strong compounds, is proposed. Under the influence of the additive, significant changes occur in the structure and optical properties of the ZnS-Ge composite, especially its first component. The IR spectroscopic data of the ZnS- B_2O_3 system indicate the absence of B_2O_3 in the coating and its accumulation in the residue after evaporation.

Table

Parameters of the evaporation of the composites, optical and operational properties of the resulting thin-film coatings

Specimen	I, A	t, min	d _{opt.} , nm	n	f·10 ³	H _m , rot.
ZnS	140	35	2450	2.12	1.69	2000
$ZnS-B_2O_3$	130	25	2500	2.33	2.54	33000
ZnS-Ge	130	20	2380	3.0	2.35	8000
ZnS-Ge-B ₂ O ₃	110	25	2380	3.0	2.62	18000
Note: I – current strength; t – time; d_{opt} – optical thickness; n – refractive						
index; $f - evaporation$ coefficient; H_m – mechanical durability						

The B_2O_3 additive has a positive effect on the optical and especially the operational properties of thin-film coatings obtained by thermal evaporation in a vacuum of composites. Thus, the strength of the evaporation current decreases significantly, which indicates an increase in the volatility of the composites, and the mechanical durability of the resulting coatings also increases (Tab.).



ORAL REPORTS

Session 4 Thin film compounds for electronic devices, nanoelectronics



Advanced polymer matrixes and nanocarriers for construction of amperometric biosensors

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Conservation and restoration of water resources is a huge problem for modern society. Some xenobiotics, apart from wastewater treatment plants, are also in the surface and underground waters, because they were only partially removed in the process of the existing technological schemes for cleaning of wastewater. One of such innovations is creation of highly sensitive biosensors for analysis of the level of wastewater pollution. The studies of micro/nanomodified polymers will lead to the creation of devices with a significantly expanded range of capabilities for detecting harmful contaminants.

The main aim of the research curried out was focused on the creation of new bio-recognizing layers based on enzymes for analytical purposes and novel polymer matrixes and electroconductive micro/nanomaterials, which can be used for effective enzyme immobilization [1-9]. Metal nanoparticles (NPs) and highly dispersed inorganic materials were used as nanocarriers of bioselective molecules. The synthesized novel polymer matrixes and micro/nanomaterials were used for the construction of biorecognition layers of new amperometric biosensors. Special attention was paid to study the possible advantages of NPs compared with their micro-analogues, in particular, possibility of direct electrochemical communication between enzymes and electrode surface in redox systems on the example of laccase. In addition, a correlation was established between the network properties of the biorecognizable layer (namely, free volume at the glass transition temperature $T_{\rm g}$ and coefficients of thermal expansion of free volume cavities in the regions below and above $T_{\rm g}$, and their difference) and biosensor characteristics (maximum saturation current, range of linearity, slope of the calibration curve, and the sensitivity of bioelectrodes) to be considered as a possible way to control the biosensor's parameters.

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Flexible in-plane thermoelectric modules based on nanostructured layers of ZnO and ZnO:In

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The rapid development of miniaturized and portable electronics requires lightweight and flexible power supply systems. Among them, flexible thermoelectric (TE) devices based on the direct energy conversion between heat and electricity, show promises to generate electricity in a ubiquitous, unintermittent and noiseless way for wearable applications. In common thin-film in-plane TE modules and assembled from these modules flexible thermoelectric generators (FTEGs), thermoelectric thin films are deposited onto flexible substrates. FTEG with a planar structure and serially connected with ohmic contacts single TE legs is the simplest of various typical structural designs of flexible thermoelectric generators. When two ends of the TE film are subjected to a temperature difference (ΔT), a Seebeck voltage (ΔV) equal to $\Delta V = -S\Delta T$ (*S* represents Seebeck coefficient) is generated.

In this study, to create flexible in-plane thermoelectric modules, we used low-temperature cheap and scalable method Successive Ionic Layer Adsorption And Reaction (SILAR) for a deposition of nanostructured ZnO and ZnO:In thin films from aqueous solutions on polyimide (PI) substrates as single TE legs serially connected with ohmic aluminum (Al) contacts. Analysis of surface morphology, crystal structure, chemical composition, optical, electrical and thermoelectric properties of ZnO and ZnO:In thin films grown via SILAR on PI substrates together with output thermoelectric characteristics of n-type thermolegs based on these films has been used to select the optimal SILAR modes for new designs of low-cost lightweight flexible thin film thermoelectric modules. Obtained flexible TE modules successfully tested for a suitability to supply electrical energy for miniature devices due to utilization the unnecessary low-potential heat at near-room temperatures. It is experimentally confirmed that the use of a zincate and sulfate solutions in the SILAR method allows to obtain nanostructured 1.4 µm thick ZnO:In and ZnO films, respectively. These films after post-growth annealing at 300 °C have Seebeck coefficients in the 70-110 μ V/K range, low resistivity ρ , and good thermoelectric power factors S^2/ρ at near-room temperatures. Especially, in the best ZnO/PI TE sample $\rho \approx 0.0015 \Omega$ m, and S^2/ρ is from 5.7 up to 7.8 μ W K⁻² m⁻¹. The in-plane TE modules based on ZnO:In/PI and ZnO/PI samples equipped with ohmic Al contacts are able to produce specific output power 0.04 and 0.09 W/m² at $\Delta T = 50$ K, respectively.
Flexible thermoelectric and photosensitive thin-film material based on nanostructured ZnO:In layer covered by nanocellulose

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With the advent of wearable device technology, fabrication of inorganic semiconductor devices on flexible organic substrates is of great interest. Among such devices, low-cost photodetectors based on wide bandgap semiconductor films have been developed in order to monitor and control the level of UV dosage and exposure of ultraviolet (UV) light that has been commonly utilised in biomedical applications, astronomy, space communication and water treatment. In particular, n-type wide-gap semiconductor zinc oxide (ZnO) and its alloys have attracted special attention because they are cheap, available, nontoxic, and thermally and chemically stable in air. The need to power up portable and wearable flexible electronics motivates the development of flexible thermoelectric (TE) materials. Thermoelectric technologies are increasingly being seen as a key to realizing self-powered electronic applications such as flexible photodetectors operating at near-room temperatures. In particular, indium doped zinc oxide (ZnO:In) thin film TE materials are feasible to convert waste heat into electricity at the level of several μW per square meter of useful area. However, ZnO and its derivatives have high sensitivity to different gases and vapors. Therefore, for stable operation of flexible photodetectors and other electronic devices based on zinc oxide, it is necessary to isolate them from the environment. In this work, we used for this purpose nanocellulose (NC) barrier coating prepared from nanocellulose suspension obtained through 2,2,6,6tetramethylpiperidine-1-oxyl (TEMPO)-mediated oxidation of a widespread plant common reed (Phragmites australis). For a deposition of nanostructured ZnO:In thin films from aqueous solutions on polyimide (PI) substrates we used low-temperature cheap and scalable method Successive Ionic Layer Adsorption And Reaction (SILAR), and thus obtained flexible thermoelectric and photosensitive thin-film material ZnO:In/PI. Thereafter, we topped surface of ZnO:In with nanocellulose suspension via drop casting method, and investigated thermoelectric and photosensitive properties of the obtained flexible material NC/ZnO:In/PI. It was found that although the NC coating leads to a certain decrease in the output TE parameters, it accelerates the photoresponse and ensures stable operation of NC/ZnO:In/PI as a photosensitive material.

Dynamic photoinduced changes of optical characteristics and effect of optical memory in amorphous As–S film-based waveguides

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Amorphous films of As–S system reveal a number of interesting photoinduced effects and are promising materials for modern optoelectronics and photonics as well as for the fabrication of elements of integrated optics [1]. Using a highly sensitive waveguide method with prism-coupling configuration, we studied photostimulated dynamic and irreversible changes of the refractive index n_f as well as photoinduced variation of attenuation parameter for optical guiding modes in As_xS_{1-x} films (0,15≤x≤0,30) under above-bandgap laser illumination (λ =480 nm). Variation of n_f was determined with an accuracy of 10⁻⁴. At the initial stage of the sample exposure to light n_f shortly decreases by a value of the order of 10⁻³ followed by a monotonous increase of n_f until a state of saturation is achieved. If the illumination is interrupted, a similar behaviour of n_f is observed (short decrease followed by a monotonous increase).

The dynamic variation of the film n_f is accompanied by a so-called stopping effect [2] consisting in a sharply increasing attenuation of a waveguide mode under continuous pumping by the above-bandgap light. Dynamics of variation of the waveguide mode attenuation is determined by the competition of two independent processes: external optical recording with a long-term (at least several hours) memory effect and an active function of the assisting waveguide mode by virtue of removal of the preceding optical record (reproduction of the preceding value of attenuation of optical modes in the waveguide stimulated by the light with λ =633 nm).

Comparison of the kinetics of the photoinduced non-monotonous changes of n_f and specific features of the stopping effect revealed a similar dynamics in their behaviour caused by the character of generation and recombination of excited electrons self-trapped on deep levels, their interaction with excitons forming a polaron potentional well. The active role of the assisting light is due to its absorption by these electrons and their transition to the conduction band.

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Energetic distribution and nature of traps in SICN amorphous films

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SiCN ternary compounds are recognized as a promising material for application in modern semiconductor electronics due its excellent high-temperature physical properties, low value of electric permittivity, high chemical, radiation and mechanical stability over a wide temperature range. Amorphous SiCN films were deposited on single crystal silicon substrates of *p*-type conductivity by plasma-enhanced chemical vapor deposition technique [1].

The films were characterized by measuring direct current conductivity, barrier capacitance and photovoltaic response in Schottky contacts deposited on the surface. The conductivity is shown to be determined by the space-charge limited (SCL) conduction mechanism. To study the states of traps in the obtained films, the SCL current was measured as a function of the bias voltage and temperature. It is shown that the experimental current-voltage characteristics consist of a sequence of power-law dependences $I \sim U^k$ with different values of k, which depends on the conditions of film deposition. According to Lampert and Mark [2], the experimental results indicate the presence of shallow and deep traps in the films under study. To explain their nature models of the local energy band in the forbidden gap with exponential and Gaussian distributions of traps were examined. The theory of SCL current predicts difference between exponential and Gaussian distributions, which should be pronounced at low and high bias voltages. However, since the current-voltage measurements are performed in a finite range of bias voltage where both distributions can give the same result. Band and trap parameters (mobility of electrons, density and energy of trap states) are estimated from the SCL current measurements. The nature of traps in the investigated films is briefly discussed. Evidences are given that traps can be attributed to dangling silicon bonds, which are inevitably present in large quantities in these films. Since little is known about defect states in amorphous SiCN films, it is also possible that dangling bonds can indirectly manifest the action of other structural defects, such as vacancies, dislocations, or impurities.

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ORAL REPORTS

Session 5 Functional crystalline materials: growth, physical properties and applications



Synthesis and characterization of new mixed layered compounds GeBi₃Te₄ and GeBi₄Te₄

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Tetradymite-like layered compounds of the $(A^{IV}Te)m(B2VTe3)n (A^{IV} = Ge, Sn, Pb; B^{V} = Sb, Bi)$ homologous series are long studied as thermoelectric materials. Discover of new functional materials – topological insulators (TIs)[1], made these chalcogenides of heavy p-elements very useful in optoelectronics, spintronics, quantum computing. Data analysis indicates that in $A^{IV}-B^{V}-Te$ systems, besides above mentioned homologous series, phases can also exist relevant to $mBi_2 - A^{IV}B_2^{V}Te_4$ homologous series[2,3].

In this paper, we report synthesis and characterization of a new mix layered GeBi₃Te₄ and GeBi₄Te₄ compounds in the Ge-Bi-Te system consisting of repetition of seven-layer GeBi₂Te₄ and two-layered Bi₂ packets in the form of -7-7-2-7-7-2- and -7-2-7-2- along the *c* axis respectively.

High purity (99.999%, Alfa Aesar) Ge, Bi, and Te elements were used to synthesize the novel mix layered polycrystalline samples. The mixture of components heated up to 800 °C and quenched in ice water. Then samples were annealed at 450 °C for 1000 h in order to reach the equilibrium state.

The synthesized ingots were investigated by powder X-ray diffraction analysis at room temperature with Bruker D2 PHASER X-ray diffractometer (CuK_{α 1} radiation) and Differential Thermal Analysis. The parameters of the crystal lattice were calculated using TOPAS V3.0 software.

The synthesized samples are compared with Bismuth and GeBi₂Te₄ compounds. Diffraction patterns of the synthesized samples have new diffraction peaks. It was determined that the novel GeBi₃Te₄ phase has rhombohedral lattice type with the a=4,3625(5)Å, c=31,381(2)Å lattice parameters in the trigonal configuration and GeBi₄Te₄ has hexagonal configuration with a=4,4071(6)Å, c=17,384(2)Å lattice parameters.

The DTA results show that newly discovered $GeBi_3Te_4$ and $GeBi_4Te_4$ phases melt with decomposition at 563 °C and 538 °C respectively.

Novel mixed layered compounds increase the probability of presence of compounds belonging to nB_2^{V} - $mA^{IV}B_2^{V}Te_4$ homologous series in the A^{IV} - B^{V} - Te system.

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Optical phonon modes and crystal structure of Hg₃S₂I₂

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Our investigation presents the decomposition of the vibrational modes for $Hg_3S_2I_2$ crystals in the center of the Brillouin zone using the group theory. Normal modes classified according to the irreducible representations for both infrared-active and Raman-active modes. According to the single crystal X-ray diffraction the $Hg_3S_2I_2$ compound crystallizes in the orthorhombic space group Imma (No. 74) with eight molecules per unit cell. The space group Imma is a symmorphic, and the group of wave vector at k=0 is D_{2h} . In Schoenflies notation, the Imma is equivalent to D^{28}_{2h} , making the relevant point symmetry D_{2h} or mmm. By using the table of irreducible representations of the crystallographic point group D_{2h} of space group Imma the contributions of all spices of atoms to normal modes of $Hg_3S_2I_2$ is analyzed. Long-wave phonons are distributed on irreducible representations of point group D_{2h} .

According to the group theory analysis, 32 normal modes are active in IR spectra and 42 modes are active in Raman spectra. The infrared-active modes have B_{1u} , B_{2u} and B_{3u} symmetries while the Raman-active modes have A_g , B_{1g} , B_{2g} , and B_{3g} symmetries. The fundamental modes of A_u symmetry are not active in both Raman and IR spectra. So the A_u modes are silent. It should be noted that modes of A and B symmetries are non-degenerate. The acoustic modes belong to representations which contain the translations vectors T_x , T_y and T_z . Internal vibrations of A_g and A_u symmetries describe the composition and symmetry of the crystal's motive. The rotations R_z , R_y and R_x have the same symmetry properties as that of the B_{1g} , B_{2g} , B_{3g} fundamental modes. They have the same symmetry properties as those of B_{1g} , B_{2g} , B_{3g} symmetries become active in Raman spectra of $Hg_3S_2I_2$ crystals.

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Development of the autonomic stations on a high efficiency thermolectric generators

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It is extremely important for future generations to reduce the amount of global energy consumed, and this can only be achieved through technological development and the use of renewable energy sources. Such sources are solar energy, wind and hydropower, in addition to the currently used energy sources. Among these various energy sources, thermoelectricity is currently becoming a common and promising alternative energy source. However, if thermoelectric coolers of cold have received a decent development and have found their commercial niche. The development of thermoelectric generators of electricity is hindered by their relatively low efficiency of converting thermal energy into electrical energy of not more than 8 %. And therefore, the main task of researchers working in this field is a sharp increase in the effectiveness of the transformation by one and a half to two times. This is what this work is dedicated to.

Temperature Dependence of Hall Coefficient in Bi₂(Te_{0.9}Se_{0.1})₃ Polycrystal

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Bi₂(Te_{1-x}Se_x)₃ solid solutions are known to be one of the best materials for use in thermoelectric devices as *p*- and *n*-type legs of thermocouples. It is known that Bi₂Se₃ compound has *n*-type conductivity and acts as an isovalent impurity for Bi₂Te₃ compound which has *p*-type conductivity. Since Bi₂Te₃ and Bi₂Te₃ have different types of intrinsic point defects, the band structure of Bi₂(Te_{1x}Se_x)₃ solid solutions can be studied only qualitatively. Typically, the change in conductivity type ($p \rightarrow n$) in Bi₂(Te_{1-x}Se_x)₃ occurs at $x \sim 0.3$ with the formation of Bi₂Te₂Se compound. The method of samples' preparation also affects the defect structure: for example, cold-pressed Bi₂(Te_{1x}Se_x)₃ polycrystals have *p*-type conductivity in the whole range of concentrations x [1]. In addition, the defects, and hence the conductivity type are influenced by such external factors as temperature *T* and the magnitude of the magnetic field *B*.

The aim of the work: the study of the Hall coefficient $R_{\rm H}$ dependence of the Bi₂(Te_{0.9}Se_{0.1})₃ solid solution on the temperature and magnetic field. Object of the research: polycrystalline Bi₂(Te_{0.9}Se_{0.1})₃ solid solution, obtained by ampoule method and annealed for 300 hours at $T = (670 \pm 5)$ K. Measurements of the Hall coefficient $R_{\rm H}$ were performed by standard *dc* method on parallelepipeds (10×3×2 mm) in the T = 80300 K temperature range at magnetic fields of B = 0.03 and 1.0 T.

The $R_{\rm H}(T)$ dependences are obtained for different values of *B* and the complex behavior of $R_{\rm H}(T)$ depending on *T* and *B* is revealed. At a small magnetic field (B = 0.03 T), the value of $R_{\rm H} > 0$ in the entire temperature range, moreover, the $R_{\rm H}(T)$ dependence is extreme with a maximum near T = 200 K. In a larger magnetic field (B = 1.0 T) with increasing temperature the sign of $R_{\rm H}$ changes from "-" to "+" near $T \sim 120$ K, and the $R_{\rm H}(T)$ dependence also has a non-monotonic character with a maximum near T = 200 K.

The non-monotonic behavior of $R_{\rm H}(T)$ in different magnetic fields is a consequence of a complex process of activation of defective states. It is assumed that the "electronic component" of $R_{\rm H}$, which dominates at low *T* and high *B*, decreases in the T = 80 - 200 K range, and the "hole component" of $R_{\rm H}$ becomes dominant. The value of the "hole component" begins to decrease at T > 200 K, which leads to the presence of a maximum on the $R_{\rm H}(T)$ dependence.

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Thermoelectric abilities of superlattices described by Fivaz model

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Now the thermoelectric properties of the superlattices described by Fivaz model are the object of intensive studying. The main peculiarity of current carriers' band spectrum of these superlattices is quasi-two dimensional. In framework of Fivaz model the motion of current carriers may be described by effective mass approximation in the layers plane and by tight-binding approximation in perpendicular direction, or along C-axis. Such band spectrum allows achieving the principal new thermoelectric properties. These properties are the high thermoelectric figure of merit, the low electric contact resistance "thermoelectric material-metal" and high anisotropy of Seebeck coefficient.

The high thermoelectric figure of merit may be achieved for so-called "transient" Fermi surface. Its' size along the C-axis is equal to the length of onedimensional Brillouin zone. If electric current and temperature gradient are parallel to layers' plane, then the efficiency of thermoelement in the electricity generation mode may achieve 35% between temperatures 300 and 500 K for optimal combination of crystal parameters. But the real layered thermoelectric alloys of Bi(Sb)-Te(Se) system have not such optimal combination of parameters, hence real efficiency of thermoelectric generating modules is not more then 5-8%.

The low contact resistance "thermoelectric material-metal" may be achieved due to effective blocking of the current carriers' scattering in the C-axis direction due to limitation of current carriers' motion in this direction. For high rate of the doping of the contact region, when the Fermi surface of thermoelectric material is transient or open, the contact resistance "thermoelectric material-metal" may achieve the so called "limit of detection", i.e. $10^{-9}\Omega \cdot \text{cm}^2$.

The big anisotropy of Seebeck coefficient, i.e. difference between Seebeck coefficients in the layers' plane and in the perpendicular direction due to the optimal combination of the band spectrum anisotropy and the current carriers' scattering anisotropy for transient or open Fermi surface may achieve 300μ V/K. It is very important for anisotropic thermoelements.

Functional Cristalline Materials on the Base Bees Products

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The physicochemical of liquid structural and characteristics and crystallized(solid) honey, depending on its thermochemical treatment during storage for a long time, were also studied. Identified 3 main factors that affect the rate of crystallization of honey is the water content, pollen content and the ratio of glucose and fructose in honey. Using a new method of low-temperature isothermal accelerated processing of honey in a microwave reactor type MWR-SPR at 50oC, and in 60 seconds, you can dissolve (decrystallize) solid, crystalline honey to a liquid state. This method reduces the time for its dissolution in the classical method by heat transfer through the wall of the reactor from hot water or electric heating from 4-12 hours at the same temperature of for 1 min, that 500 times faster.

It is proved that low-temperature, isothermal, accelerated processing in a microwave reactor type, maintains a high diastase number according to Gotha, in the range of 10-11. The content of undesirable hydroxymethylfurfural did not exceed 3-6 mg / kg of honey, which meet the requirements of DSTU for honey. And consumer organoliptic indicators of honey in a liquid aggregate state remain, within 1 year. At the same time, with the classical method of crystallization-dissolution of honey, the classical method of heat transfer through the reactor wall, these figures are much worse, the diastase number of Goethe units decreases to 0-6, and the content of toxic hydrosimethylfurfural increases to 12-18 mg / kg, which considerably exceeds admissible norms of DSTU 4497 natural honey.

Light microscopy showed that the number and size of pollen particles in liquid decrystallized honey decreased by 10 times, and the size of glucose and sucrose crystals after treatment decreased by 5 times. At the same time, the analysis of the molecular weight distribution of sugar macromolecules in honey by the method of angular distribution of the laser beam (NANODS CILAS) showed a decrease in their average size by 2 times. On the basis of samples of dissolved (decrystallized) liquid honey, according to the described technology, a preventive chewing gum was created for the treatment of periodontal gingivitis, periodontitis and periodontitis. Clinical studies of chewing gum samples based on a composition of liquid, caramelized honey, wax and propolis, which were conducted at the Research Center for Molecular Microbiology and Immunology of Mucous membranes of Uzhgorod National University, showed a positive result in 72.5% of patients with periodontitis.

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Feasibility of high performance in *p*-type GeTe based compounds

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GeTe crystallizes with a strong deviation from the stoichiometric composition (in the direction of Te excess), which results in a growth of free carrier concentration (holes) up to $p \sim 10^{21} \text{ cm}^{-3}$. Such concentration is too high from the viewpoint of thermoelectric applications (maximum value of the figure of merit Z). The work demonstrates the possibility of increasing the thermoelectric efficiency of the GeTe-based material, used for the *p*-type leg of the thermoelement over the temperature range of 600-825 K. The samples were prepared using Spark Plasma Sintering (SPS) technique. A systematic analysis of thermoelectric properties for $Ge_{1-x}Pb_xTe$ alloys (x up to 5 at.%) has been performed. An increase in the lead content in Ge_{1-x}Pb_xTe alloys creates two parallel processes. The first process is a decrease of the lattice thermal conductivity κ_{lat} , which acts up to $T \approx 550$ K, when the lead content in Ge₁₋ $_{x}Pb_{x}Te$ alloys increases up to 5 at. %. However, the main process is to reduce deviation from the stoichiometric composition, which consequently leads to lower hole concentration p. Therefore, at a high temperature of $T \ge 550$ K Fermi level $E_{\rm F}$ is approaching the edge of the valence band $E_{\rm v}$. As a result, the thermoelectric dimensionless figure of merit ZT increases up to 1.1 at the temperature of 825 K.

Calculation of Stable Geometric Configuration of CdS

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Cadmium chalcogenides and structures based on them have been of considerable scientific interest in recent decades. The optimal structures for their application are heterosystems. The advantage of CdTe thin film compounds is the ability to generate and accumulate carriers. Forming of layer structures, in order to increase efficiency, serve to improve the properties of finite devices.

The use of CdS is caused by the ability to absorb in the ultraviolet (UV), visible and near infrared (NIR) region, optical nonlinearity. The high value of the band gap width of the CdS layer contributes to the good absorption of a wide range of optical spectra [1]. The disadvantage is the low ability to accumulate the generated charge. To eliminate this shortcoming, this layer is combined with other materials, most often with CdTe. That is why there are a large number of studies of different characteristics of the CdS / CdTe type heterosystem. The efficiency of such systems at 50 nm CdS layer thickness is 15.8% [2]. Accordingly, for such a small thickness, the basic properties will be determined by the structural characteristics of their surface.

The compound is characterized by the ability to crystallize in two modifications - sphalerite and wurtzite lattice, which depends on the synthesis conditions and annealing temperature [3]. It is important to determine theoretically the conditions for obtaining of predetermined crystal lattice.

Thin CdS films were obtained by open evaporation in vacuum. The PC Gamess (US) [4] was used to calculate the stable crystal structure and thermodynamic parameters of crystalline CdS. Calculations were performed using density functional theory based on the Stevens-Bash-Krauss-Jacien-Kundari parameterization (SBKJC).

The values of the Gibbs energy for the sphalerite and wurtzite modifications were compared to find the stable crystallographic positions of the atoms and the temperature of the sphalerite-wurtzite phase transition. It is determined that the transition from cubic to hexagonal modification occurs at 320.74 K.

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Point defects in bromine-doped cadmium telluride crystals

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Cadmium telluride is a promising material for the manufacture of highly efficient optoelectronic devices and ionizing radiation detectors. It is possible to improve and stabilize the characteristics of the material by doping with various impurities, in particular with bromine. To develop a scientifically based technology for CdTe:Br, reliable information about its defect subsystem is required.

In this work, the formation of point defects in bromine-doped cadmium telluride crystals has been described using quasi-chemical reactions, and based on this, the dependences of the concentrations of point defects and free charge carriers on technological factors of two-temperature annealing have been calculated.

It has been shown that the doping effect of bromine impurity in CdTe crystals is associated with substitutional defects and their complexes with intrinsic point defects $(2Br_{Te}^+V_{Cd}^{2-})^0$, which are dominant in the entire investigated range of technological parameters of annealing and determine the concentration of free charge carriers in the material.

We have calculated isothermal and isobaric dependences of the concentration of free charge carriers (electrons *n* and holes *p*) and dominant intrinsic and impurity point defects (doubly charged cadmium $\begin{bmatrix} V_{Cd}^{2-} \end{bmatrix}$ and tellurium $\begin{bmatrix} V_{Te}^{2-} \end{bmatrix}$ vacancies; interstitial cadmium $\begin{bmatrix} Cd_i^{2+} \end{bmatrix}$ and tellurium $\begin{bmatrix} Te_i^{2-} \end{bmatrix}$; singly charged bromine on tellurium site $\begin{bmatrix} Br_{Te}^+ \end{bmatrix}$ and complexes $(2Br_{Te}^+V_{Cd}^{2-})^0$) in bromine-doped cadmium telluride crystals under conditions of two-temperature annealing in cadmium vapor.

The equilibrium constant for the formation of complexes of impurity substitutional defects with intrinsic point defects $(2Br_{Te}^+V_{Cd}^{2-})^0$ has been determined.

The calculation has shown that the electron concentration is practically independent of the annealing temperature and, at the same time, linearly depends on the cadmium vapor pressure, which is in good agreement with experiment. This confirms the adequacy of the chosen model of defect formation in bromine-doped cadmium telluride crystals, in which the dominant defects are singly charged impurity atoms on the tellurium site Br_{Te}^+ and complexes $(2Br_{Te}^+V_{Cd}^{2-})^0$.

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Effect of fast electron irradiation on CdZnTe crystals

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The effect of fast electron irradiation with doses $\Phi = 10^{13} - 10^{15}$ e cm⁻² on the spectral characteristics of low-temperature photoluminescence LTP (T=77K) of p-type Cd_{1-x}Zn_xTe crystals (x = 0.05) was investigated. The LTP spectra of the unirradiated CdZnTe crystals consist of an impurity-defect band D (hv_m =1.43-1.58 eV) and an exciton band (hv_m = 1.607 eV) due to radiative recombination of excitons bound on neutral donors D⁰X and free excitons FE (Fig., curve 1). It is established that with increasing of Φ the intensity of the impurity-defect band I_D decreases, and the exciton I_D⁰_X changes nonmonotonically. At irradiation doses $\Phi = 10^{13} - 10^{14}$ e·cm⁻² (Fig., curve 2), a





decrease in PL intensity in both the impurity and exciton regions of the spectrum is observed. Irradiation with a dose $\Phi = 10^{15} \text{ e} \cdot \text{cm}^{-2}$ leads to a further decrease in the intensity of the impurity band PL and a sharp increase in the intensity of the exciton band (Fig., curve 3). The decrease in the intensity of impurity and exciton PL at doses $\Phi = 10^{13} - 10^{14} \text{ e} \cdot \text{cm}^{-2}$ is caused by the generation of radiation-stimulated defects, which are effective centers of

nonradiative recombination. Increasing the radiation dose to $\Phi = 10^{15} \text{ e}\cdot\text{cm}^{-2}$ leads to the accumulation of radiation-stimulated defects and their interaction with growth defects. The increase in the PL intensity of the exciton band may be associated with: a) the process of radiation-stimulated structural ordering (the effect of small doses); b) restructuring of impurity-defect complexes under the action of irradiation - activation of neutral impurity-defect centers of donor type and / or formation of impurity-defect complexes of donor type.

Features of structural, thermodynamic, energetic, kinetic and magnetic characteristics of Lu_{1-x}Zr_xNiSb solid solution

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Thermoelectric materials based on half-Heusler phases demonstrate a high efficiency of conversion of thermal energy into electricity [1]. Therefore $Lu_{1-x}Zr_xNiSb$ solid solution obtained by doping of LuNiSb compound with Zr atoms by substitution Lu atoms at position 4a was investigated. In this case, the structural defects of a donor nature are generates in semiconductor since Zr $(4d^25s^2)$ has more *d*-electrons, than Lu atom $(5d^16s^2)$.

Modeling of the electronic structure of *p*-LuNiSb showed that only in the presence of vacancies in the crystallographic positions 4a and 4c of the Lu and Ni atoms appears a band gap ε_g . In this case, structural defects of acceptor nature are generated in the crystal, and acceptor levels appear in the band gap ε_g . Structural studies of Lu_{1-x}Zr_xNiSb revealed the nonmonotonic change of the lattice parameter values a(x): at concentrations $x = 0-0.02 \ a(x)$ values increase, and at x > 0.02 they decrease monotonically. We assume that increase of a(x) is due to the occupation of vacancies in position 4a by Zr atoms and in position 4c simultaneously by Ni and Zr atoms. In this case the structural defects of donor nature are generated and donor levels appear in the band gap. At the same time the structural defect of the acceptor nature (vacancy) in position 4c and the corresponding acceptor level (band) ε_A^1 disappear.

Doping of *p*-LuNiSb with the lowest concentration of Zr atoms (x = 0.01) changes the behaviour of the temperature dependences of the resistivity ρ and the thermopower coefficient α and the type of the main current carriers. The increase of the temperature dependences of the resistivity $\rho(T,x)$ of Lu_{1-x}Zr_xNiSb indicates that the Fermi level ε_F has left the band gap ε_g and is located in the conduction band, as indicated by the negative values of the thermopower coefficient $\alpha(T,x)$ at all concentrations and temperatures. The investigated Lu_{1-x}Zr_xNiSb solid solution is a promising thermoelectric material.

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Investigation of semiconductive thermoelectric material Er_{1-x}Sc_xNiSb

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The structural, energetic, kinetic and thermodynamic characteristics of the semiconductive solid solution $\text{Er}_{1-x}\text{Sc}_x\text{NiSb}$ in the ranges T=80-400 K, x=0-0.10 were studied. It is experimentally established that at the studied concentrations of $\text{Er}_{1-x}\text{Sc}_x\text{NiSb}$ the main carriers of electricity in the semiconductor are holes. It was shown that doping of *p*-ErNiSb by Sc atoms introduced by substitution of Er atoms in position 4a is accompanied by the occupation of vacancies in the compound at crystallographic position 4a, which leads to the reduction and elimination of structural defects of acceptor nature and the corresponding acceptor band AEr. In this case, structural defects of donor nature are generated in position 4a and an impurity donor band DSc appears. The concentration ratio of the ionized acceptors and donors generated in $\text{Er}_{1-x}\text{Sc}_x\text{NiSb}$ determines the position of the Fermi level F and the mechanisms of electrical conductivity.

The energy expediency of the existence of Er_{1-x}Sc_xNiSb substitutional solid solution up to the concentration $x \approx 0.10$ was established by modeling the variation of free energy $\Delta G(x)$ values (Helmholtz potential). At higher Sc concentrations, x > 0.10, there is stratification (spinoidal decomposition of phase). It is shown that in the structure of *p*-ErNiSb semiconductor there are vacancies in positions 4a and 4c of Er and Ni atoms, respectively, generating structural defects of acceptor nature. The number of vacancies in position 4a is twice less than in position 4c. This ratio also remains for p-Er_{1-x}Sc_xNiSb. Doping of *p*-ErNiSb semiconductor by Sc atoms by substitution of Er atoms is also accompanied by the occupation of vacancies in position 4a. In this case, Ni atoms occupy vacancies in position 4c, which can be accompanied by the process of ordering the p-Er_{1-x}Sc_xNiSb structure. Occupation of vacancies by Sc and Ni atoms leads to an increase of the concentration of free electrons, an enlarge of the compensation degree of semiconductor, which changes the position of the Fermi level ε_F and the mechanisms of electrical conductivity. The investigated $Er_{1-x}Sc_xNiSb$ solid solution is a promising thermoelectric material.

The Electronic and Magnetic Properties of the ZnSe:T Crystals (T = Ti, V, Cr, Mn, Fe, Co, Ni) with a Cationic Vacancy and Under Pressure

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The pressure-dependent parameters of the electronic energy spectrum of ZnMnSe material without and with a vacancy are shown in Fig. 1. Without a



Figure 1. The electronic energy band parameters E_v , E_f and E_c in the ZnMnSe material versus the 2×2×2 supercell lattice constant.

vacancy, at pressures of 0, 22 and 51 GPa, the optical band gaps coincide with the fundamental ones, and their values are 1.04, 1.96 and 1.85 eV for spin up, and 1.20, 2.21 and 1.95 eV for spin down, respectively. The magnetic moments are equal to 5 μ B. With a vacancy, the picture changes radically. The Fermi level for both spin orientations is located at the top of the valence band. At pressures of 0, 20 and 49 GPa, the values of pseudogaps 1.03, 1.96 and 1.85 eV for spin up, and 1.20, 2.07 and 1.55 eV for spin down, respectively. The values of the magnetic moments of the supercell at these values of pressure are equal to 4.16, 4.2 and 4 μ B, respectively.

The electronic structure of the material ZnCrTiSe obtained with and without the strong correlation of Cr and Ti 3d electrons

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The work is devoted to comparative study of the spin-polarized electronic structure in a doped crystal ZnSe:Cr:Ti. The electronic energy bands and density of states have been evaluated with two approximations of the exchange-correlation potential, namely the conventional GGA-PBE and hybrid functional PBE0. The first approach corresponds to the mixing parameter $\alpha = 0$, and the second one employs the value $\alpha = 0.25$. The hybrid functional makes it possible to take into account the strong correlations of 3d electrons by removing the self-interaction error of the latter.



Fig. 1 – The spin-resolved electronic structure (a,b) and DOS (c) of the ZnSe:Cr:Ti crystal, obtained with a mixing parameter $\alpha = 0.25$.



Fig. 2 – The spin-resolved electronic structure (a,b) and DOS (c) of the ZnSe:Cr:Ti crystal, obtained with a mixing parameter $\alpha = 0$.

Comparing Figs. 1 and 2, we conclude that taking into account the strong correlations of 3d electrons in the PBE0 functional leads to significant changes in the electronic structure. Without the strong correlations (Fig. 2), the levels of 3d electrons of Cr are localized in the vicinity of the Fermi level, while with the correlations, they are below the Fermi level by more than 1 eV.

Properties of materials for ResistiveRAM (First principles calculations)

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Resistive switching random access memory (RRAM) is being considered as a next-generation non-volatile memory with promising potential advantages, such as scalability, simple structure, fast operational speed, excellent endurance, long retention and low power consumption. Various material systems including inorganic metal oxides are popular candidates for RRAM fabrications.

Phase-change memory technology relies on the electrical and optical properties of certain materials changing substantially when the atomic structure of the material is altered by heating or some other excitation process. Moreover, phase-change memory based on GST is scalable, and is therefore a candidate to replace Flash memory for non-volatile data storage applications.

The paper proposes the calculation of the characteristics of the electronic subsystem for different materials used as a working layer of RRAM.

Thus, the calculation by methods of the theory of electron density functional and pseudopotential from the first principles of characteristics of the electronic subsystem of the working layer RRAM, built on the basis of ZnO with oxygen vacancies, is proposed. The spatial distributions of the density of valence electrons and their cross sections within the cell, the distribution of the density of electronic states, and electric charges in the vacancy region are calculated. It is studied how changes in the electronic subsystem of objects affect the change of their properties from non-conductive to conductive, which gives an idea of the switching mechanism.

SiGe epitaxial films with dislocations with Ag doping regions these objects are calculated with such methods as electron density functional and first-principles pseudopotential based on own program code. [1]

GeTe/Sb₂Te₃ interfacial phase-change memory (IPCM) are studied.

The electronic structures of RRAM based on HfO₂, charge transfer of atoms, and the interaction between dopants and own atoms are studied too.

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ORAL REPORTS

Session 6 Innovative methods for teaching



Perspectives of nanotechnology in higher education

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One of the most relevant areas in science and technology is currently nanotechnology. The main advantages of nanotechnology its multi-disciplinary nature, which gives nanotechnology products a wide space for application [1, 2].

The development of the science of nanostructures and nanotechnology will make it possible to obtain nanomaterials with qualitatively new properties in the field of microelectromechanical systems. If they are used together, it will be possible to further improve existing technologies in the fields of engineering, electronics, and molecular electronics, and this will also provide a basis for creating new ones materials [3, 4].

To develop new promising nanomaterials and study their properties requires highly qualified personnel in the field of nanotechnology and microelectromechanical systems. Therefore, the training of relevant specialists in higher education institutions is an important task today [5].

In discussing this topic, we analyzed the use of computer programs to study nanoobjects during training. We also considered the possibility of introducing new interdisciplinary courses related to the development of nanotechnology in the educational process of higher education.

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Features of Studying the Topic: "Fundamentals of Practical Astronomy" Using the Virtual Planetarium Stellarium

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The subject "Astronomy" in secondary schools is designed to form general cultural competencies and scientific worldview [1]. Observations of celestial bodies are of great importance here. For their quality performance, students must have a thorough knowledge of the celestial sphere, constellations, celestial coordinates, the vigorous motion of the Sun and planets. Since the time of classes at school falls on the light part of the day, the teacher can demonstrate the starry sky only with the help of technical means.

Not every school is equipped with a planetarium to demonstrate the starry sky, so the only way out is to use the virtual. One of the best virtual planetariums is Stellarium [2]. He has many different resources that can be used in the study of "Fundamentals of Practical Astronomy" [3].

The paper presents the results of using the Stellarium program in "Astronomy" lessons at school, when studying the topic "Fundamentals of Practical Astronomy". The method of using the virtual planetarium is offered and the comparative characteristic of results of training of the considered theme on use of the Stellarium program and without it is made.

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Application of "Pedagogical workshops" technology at studying of chemistry

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Teachers have always been concerned about the question how to overcome students' reluctance to learn, how to prevent a decline in the prestige of knowledge in society? Modern pedagogy faces the task not only to equip the student with specific knowledge, skills and abilities, but also the ability to acquire them independently. In this regard, there is an active search for technologies and techniques that allow to solve the problem. One of the pedagogical technologies that allows us to meet the challenges of today is the technology of "Pedagogical Workshops" created in France in the 1920s by psychologists Paul Langevin, Henri Vallon, Jean Piage and others. This technology began to be used in domestic pedagogy only at the end of the 20th century. A pedagogical workshop is a form of children and adults teaching that creates conditions for each participant to ascend to new knowledge and new experience through independent or collective discovery. The basis of discovery in any field of knowledge, including chemical science, in the workshop is an independent creative activity of each and awareness of the laws of this activity. Therefore, the purpose of this study was to assess the effect of the technology of pedagogical workshops on the level of independence and creativity of students in chemistry lessons.

Students of two 8th grades, divided into experimental and control groups, took part in the pedagogical experiment. The distribution was completely uniform (in terms of the level of preparation of students). This made it possible to exclude from the experiment the possibility of error due to factors not related to the study.

For the research we developed and conducted a lesson on the technology of "Pedagogical workshops" in experimental groups of 8th grades on the topic "Characteristics of a chemical element by its placement in the periodic table and the structure of the atom", and developed and conducted a lesson in control groups on classical methods. The stages of the lesson were closely interrelated. The purpose of the lesson is achieved in both classes and both groups. It is shown that the application of non-traditional methods of new material learning, the main emphasis of which was placed on the independent work of students, made it possible to increase the determinant indicators of the effectiveness of learning material. The average score on the sample in two different experimental groups increased by 12 and 14%, and the quality of learning material by 20%. Although the positive impact of technology on students with different levels of training was not the same. Thus, for eighth-graders with a sufficient level of preparation, the application of the method was justified, as it allowed to arouse interest in the problem, to intensify the work of students in the classroom, which had a positive impact on the results of mastering the topic. Whereas for students with a lower level of academic achievement, this method did not give a positive result.

Educational and methodological support of the course "Physical foundations of information technology"

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The discipline "Physical foundations of information technology" belongs to the list of disciplines at the educational level "bachelor", offered within the cycle of professional training of students. It is designed to study the physical phenomena, techniques and technologies that underlie the work of modern computers. Magnetic phenomena and physics of semiconductors, their role in devices for recording, reproduction and storage of information are considered.

Information technologies are defined as an interconnected set of tools and methods used for storage, processing and issuance of information

It provides students with the formation of research professional-oriented competence and is aimed at studying the theoretical and practical issues of the use of physical phenomena in computer technology and information technology.

The task of our study is to develop methodological foundations for teaching the discipline "Physical foundations of information technology in specialties – 014 "Secondary education (Physics)", "Secondary education (Computer Science)", "Secondary education (Computer Science, English)", "Secondary education (Mathematics)" for PR – bachelor.

As a result of studying the discipline, students must know the content and structure of the course, the prospects for the application of new magnetic, semiconductor, optical and other physical methods. The development of these methods will significantly increase the amount of memory, computer speed and its peripherals for future generations.

The introduction of the discipline "Physical foundations of information technology" in the educational process in a number of specialties served as the basis for the creation of methods of its teaching. " which includes - lectures, practical classes and independent work of students ..

Thus, we can say that the method used in teaching the discipline, which considers the physical foundations of information technology, gives good results.

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Methodical support of teaching the discipline "Geographic information systems and technologies"

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Recently, research on the methods of teaching geoinformatics and geoinformation systems has been conducted in Ukraine. However, their results are poorly systematized and aimed at solving production problems and tasks. The task of our study is to develop methodological foundations for teaching the discipline "Geoinformation Systems" and testing of the developed methodology.

At the Vasyl Stefanyk Precarpathian National University, courses related to the use of geographic information technologies are taught in the specialties "Geography", Secondary Education (Geography), "Earth Sciences", "Ecology and Nature Management", both for bachelors and and for masters.

Educational programs are built on a two-tier system - "bachelor - master" and determine the division of the block of disciplines into stages: preparatory stage - gaining skills in working with a personal computer and the use of free programs; the first stage - the use of acquired knowledge and skills in the study of courses on mathematical modeling, processing of raster and vector images, digital cartography; the second stage - studying the structures of spatial data, learning the basics of GIS technologies; the final stage is the creation of a GIS project.

The introduction of GIS in the educational process in a number of specialties served as the basis for the creation of methods for teaching the discipline "Geographic Information Systems and Technologies" ...

In the considered domestic and foreign sources on this topic, much of the literature describes the use of GIS for teaching geography in high school and high school. You can also find research related to the use of GIS and the introduction of geographical content in solving applied problems [1-2].

The result of the application of methodological bases in the teaching of geoinformatics and geoinformation systems are projects of different directions.

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Use of a Hand-held XRF Instrument to Determine Rare Earth Element Concentrations

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Large geologic concentrations of rare earth elements (REEs) are uncommon, but these elements are extremely important as components for hightechnology applications. The main current supply of rare earth compounds comes from China, but a few new mining ventures now exist in the United States. The US Department of Energy has also driven the discovery of additional sources containing relatively high concentrations of REEs, mostly from coal-associated materials. Sampling and analysis of coal, rock, drilling cores, acid mine drainage (AMD) sediments, and clays associated with coal seams provided the data in this study. However, the results apply to other sources of rare earth containing materials as well.

Samples were collected at various active mining locations. These samples were later crushed and sieved to a final particle size of $125 \,\mu$ m. Portions of the resulting powders were then packed into plastic cups for XRF analysis. The XRF instrument software had been modified previously to have the capability of detecting lanthanum (La), cerium (Ce), praseodymium (Pr), and neodymium (Nd); the capability to detect scandium (Sc) and yttrium (Y) was already available given that they are lighter elements than the lanthanides. The sample cups were placed in a portable stand that accommodated the XRF instrument, and the instrument was connected to a laptop for data collection.

The original sample collection included 239 samples. Of these samples, 78 were selected for induction coupled plasma – magnetic spectroscopy (ICP-MS) analysis, since this is believed to be the preferred method for REE analysis. The Y concentration determined by ICP-MS analysis was first compared to the heavy rare earth element (HREE) concentration determined by ICP-MS analysis, which provided an exact correlation. HREEs represent those lanthanides from europium (Eu) to lutetium (Lu) including Y. Since HREE concentrations generally represent 15%-20% of the total REE concentration, it's possible to estimate the total REE concentration knowing the Y concentration. In order to do this, the Y concentration obtained by ICP-MS analysis, which provided a reasonable correlation. A compilation of the data then allowed the total REE concentration to be estimated to within $\pm 40\%$. The relative cost and expediency of ICP-MS analysis analysis thus offers an individual the ability to quickly determine a sample's value in the field using a hand-held instrument.

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Formation of global competence of students in physics lessons

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The digital age has created a society without borders, a global society. Therefore, today there is a need to learn to live and work in such a globalized world, to have global competence.

Global competence in domestic education was actively discussed in 2018, when a new section based on the subject of studying local, global and culturally significant events was introduced in the international PISA test, in which Ukraine also participated; understanding other people's worldviews; ability to take measures for collective well-being and sustainable development. The tests tested students' ability to critically evaluate news about global issues, their understanding of external influences on their worldview, and their ability to communicate with others in intercultural contexts.

The widespread use of distance technology for learning and work has shown that global competence is needed by our students who already live in a global world. Scientists identify the knowledge, skills and value components of global competence. The structural components of global competence overlap with the components of key competencies defined by regulations (*Fig.1*).



Fig.1. Components of global student competence.

Global competence is formed in the process of implementing cross-cutting content lines that are in the content of the subject of physics. The introduction of cross-cutting content lines is an appropriate interpretation of the content of education and does not involve expanding or deepening educational topics.



POSTER REPORTS Session 1 Thin films technology (metals, semiconductors, dielectrics, conductive polymers) and their research methods



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Local strain distribution in diamond crystals defined by the Fourier transformations of Kikuchi patterns

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Experimental studies of a set of 6 synthetic diamond crystals, grown under different conditions are presented. Investigations were carried out using a Zeiss EVO 50 XVP scanning electron microscope (Carl Zeiss, Germany) equipped with a CCD detector.



Fig. 1. Clustering of the studied diamond crystals based on their deformation parameters in the coordinate system ($\sigma_{\varepsilon}, M_{\varepsilon}$).

The prospect of using a new of analysis of electron method diffraction backscatter patterns is shown. It is proposed to determine the deformations of local regions of synthetic diamond crystals on the basis of normalized profiles of Kikuchi band intensity and normalized parameters of the energy Fourier spectrum without the use of reference image [1]. The use of normalized characteristics allowed to determine the values of deformations not only for areas of one crystal, but also for different crystals. In particular, it provides the possibility of analyzing diffraction images intensity profiles of

different widths, as well as the independence of the parameters of the energy spectrum from instrumental factors (the influence of noise and the average background of the image).

K-means clustering method in the space of deformation parameters of the studied diamond crystals in the coordinate system (σ_{ε} , M_{ε}) using the Euclidean distance between the points is performed (fig. 1).

[1]. Fodchuk I.M., Ivakhnenko S.A., Tkach V.N., Balovsyak S.V., Borcha M.D., Solodkii N.S., Gutsulyak I.I., Kuzmin A.R., Sumaryuk O.V. Local strain distribution in synthetic diamond crystals, determined by the parameters of the energy spectrum of the Kikuchi patterns. Journal of Superhard Materials. 2020. – Vol. 42, N_{21} . – P. 1-8.

Electrodeposition of molybdenum carbide thin films onto semiconductor materials surface

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A thermodynamic, corrosion, potentiometric and voltammetric study of the behaviour of semiconductor abrasive material (silicon and boron carbides) in halide, halide-oxide and oxide melts has been carried out. To account for the rise of surface conductance in carbide crystals when they are in contact with melts of definite composition, a concept of electrochemical potential and equilibrium due to redox processes occurring at the diamond melt interface is developed. To elucidate the mechanism of appearance of conduction, we studied (chemical and electrochemical) interactions occurring at the silicon (boron) carbide ionic melt interface. The deposition of metal-containing thin films on the surface of abrasive materials is an efficient method of increasing their performance.

Investigations were carried out into the high-temperature electrochemical deposition of molybdenum carbide thin films from ion melts in relation to temperature, cathodic current density, and process time, and attention was also given to the relations hips of these parameters with the deposition rate and the strength and service properties of abrasive materials. In electrochemical metallizing, grains of abrasive materials (silicon and boron carbides) are held in melts of an equimolar mixture of sodium and potassium tungstates with additions of molybdenum oxides (VI) and lithium carbonate at 800-900°C and a cathodic current density of 10-200 A/m². Under these conditions electrical conductivity of the surface of abrasive materials increases and the surface plays the role of an active substrate for high-temperature electrochemical synthesis. At temperatures below 800°C, metallizing does not take place because powder deposits of the molybdenum carbide form. The coating consists of a light-grey, finely crystalline, continuous deposit. Its integrity can be clearly seen on cleaves. X-ray diffraction patterns of the surface layer of specimens with coatings contain strong lines of molybdenum carbide.

The molybdenum carbide was deposited on the grain of silicon and boron carbides 40- and 16 min size, respectively, at 900°C, cathodic density 50, 100 and 200 A/m², for 15, 30, 45, 60 and 90 min. The extent of metallizing of the grains depends strongly on the cathodic current density and electrolysis time with an increase of these parameters the deposition rate increases. As a result of deposition of molybdenum carbide the coefficient of the fracture load of the grains of the silicon and boron carbides was equal to 1.5-2.5, the capillary of the SiC grains increased 3.4-4 times, and that of the boron carbide 2.3-2.5 times.

Electrochemical and corrosion behavior of titanium coated by molybdenum carbide thin films

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Thin Mo₂C films were precipitated on the surface of the VT 1-0 grade titanium by the method of high-temperature electrochemical synthesis from Na₂WO₄–5 mol. % MoO₃–10 mol. % Li₂CO₃ melt at temperature 800-900°C and cathodic current density 0.4-1.2 kA/m² on air. Maximum thickness of coating were 50 microns.

Corrosion tests of Ti before and after electroplating by thin Mo₂C films were carried out in sulfuric acid solution (9.5 mol. %) at 70-80°C observing time dependences of potential and corrosion rate. Ti corrosion potential increases essentially after coating deposition, from – 0.59-0.61 V to – 0.26-0.31 V (*versus* standard hydrogen electrode), turning to Ti passive-active potential area and not reaching potential of Mo₂C corrosion only by 0.02-0.04 V. Average rate of Ti dissolution from coated sample is constant and makes 0.005-0.01 g/(m²·h), whereas Ti dissolution rate at the free corrosion potential is equal to 19.1-19.3 g/(m²·h). As the result of coating deposition, Ti dissolution rate decreases by a factor of 2000-4000. Dissolution rate of uncoated Ti at the equilibrium potential of samples with Mo₂C coating (300-310 mV) is equal to 1.50-1.55 g/(m²·h).

Free Ti corrosion potential is equal to -0.59-0.61 V. It is characterized by the active dissolution area with rather low critical potential of passivation (-0.27-0.29 V) and with high critical current. At potential values being higher than critical passivation potential, Ti is passivated. For Mo₂C sample, the area of active dissolution is absent, and sample is passive up to the point of overpassivation potential. The curve of Ti anodic polarization with Mo₂C coating is similar to the curve of Mo₂C sample and practically coincides with it at polarization higher than 0.1 V.

According to cathodic polarization curves, efficiency of cathodic processses on Mo_2C and on Mo_2C coated Ti samples is much higher as compared with uncovered Ti ones. Mo_2C cathodic curve intersects with the anodic curve in the very beginning of active-passive area. Therefore, at the commensurable areas, Mo_2C cathode is unable to complete passivation of the Ti anode. The cathodic curve of Mo_2C coatings intersects with Ti anodic curve in the immediate proximity to passive area. Therefore, coating is more efficient as the cathode.

Structure of thick yttrium iron garnets epitaxial systems grown under different growth conditions

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We report the investigation of the set of iron-yttrium garnet thick films of different thicknesses doped with lanthanum. The influence of changes in growing parameters on the physical and technical characteristics of films as magnetic materials of high-frequency electronics and on the parameters of the crystal structure and distribution of film defects is investigated by complex of X-ray diffraction and other methods.

Epitaxial YIG films were grown by the method of liquid-phase epitaxy on substrates of gallium-gadolinium garnet with orientation 111 in SRC "Carat". Technological processes were performed on an upgraded Garnet-3 facility (LPAI, France). Samples of nominal composition YLaFeO were obtained from a solution-melt based on PbO-B₂O₃. The main attention is paid to the study of films with thicknesses from 80 to 125 μ m. In addition, the characteristics of thick films are compared with referent thin films of different thicknesses. The temperature of the melt solution was maintained at an appropriate level with a high accuracy of ± 0.1 °C in the range of 600...1200 °C. Molar ratios of the components were used to calculate the component composition of the films in the process of growing by the method of liquid-phase epitaxy. Such parameters as growth rate, temperature of garnet-forming components and their molar ratios were adjusted during the growth process.

The crystal structure of YIG films was studied by AFM and highresolution X-ray diffractometry. The dominant types of microdefects and their parameters were determine analyzing reciprocal space maps (RSMs) and rocking curves. Correctness of defect structure model is confirmed by RSM simulation, based on Krivoglaz kinematic theory combined with Monte Carlo method. MFM was used to investigate YIG magnetic characteristics. The width of ferromagnetic resonance (FMR) line, amplitudes and fluctuations of the MFM signal were also determined and analyzed for complex study of films parameters.

Effect of oxygen flow rate on properties of multilayer aluminium-doped indium saving ITO thin films

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Multilayer aluminum-doped indium saving indium-tin oxide (ITO) thin films have been designed and fabricated by sputtering method. Thin films consisted of very thin layer of conventional indium tin oxide (In_2O_3 -10 mass % SnO₂) (12 nm) and aluminum-doped indium saving indium-tin oxide layer (138 nm) with reduced to 50 mass % In_2O_3 content. Thin films were deposited in mixed argon-oxygen atmosphere onto glass substrates preheated at 523 K under the rotation of the substrate holder in order to obtain a homogeneous deposition. Obtained films were heat treated at 523 K.

It was revealed that volume resistivity of multilayer thin films increased with increasing oxygen flow rate. Such increase was observed for both asdeposited and heat-treated films. The lowest value of volume resistivity was observed for as-deposited multilayer thin film sputtered in pure argon (445 $\mu\Omega$ ·cm). Volume resistivity of multilayer thin films showed significant (in 4.6 times) decrease in comparison with single layer aluminum-doped indium saving ITO deposited under the same conditions.

Optical transmittance of as-deposited multilayer aluminum-doped indium saving ITO thin films increased when oxygen was added to sputtering gas (an average transmittance larger than 90 % in the visible range was observed).

Results of X-Ray 2θ scans reveal that both as-deposited and heat treated multilayer aluminum-doped indium saving ITO thin films show $In_4Sn_3O_{12}$ structure.

Fractal analysis of X-ray moiré images created by a set of concentrated forces

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The development of X-ray dynamical theory now allows to carry out the necessary numerical simulations of moiré images with predetermined deformation field. With this approach, the analysis of experimental moiré images can provide the necessary quantitative information about the sources of residual or active deformations and their distribution, as well as the nature of their possible interaction.

The use of simulations with a certainly distributed sets of concentrated forces allowed to investigate the influence of long-period or localized deformation fields on diffraction and interference processes of X-waves in *LLL*-interferometers.

In this paper we considered new approaches to the analysis of moiré intensity distributions based on the Fourier energy spectrum method. Different sensitivity to the distribution shape of local sources of deformation in low and high frequency ranges of radial distributions of moiré images energy spectra creates new opportunities to determine not only the total magnitude of deformation, but also their spatial distribution in the crystal.



Fig. 5. – Fractal spectral dimension for moiré forces (Fig. 3), obtained depending on L_r . S1 – moiré forces without and S2 – with phase moiré at $\Lambda = 1200 \ \mu m$, Z1800 at $\Lambda = 1800 \ \mu m$.

algorithm The of the dimension fractal value calculation is even more informative. It is based on Fourier transforms of linear profiles of moiré intensities, obtained in different directions. The similarity of differentperiod structures is better seen in comparison with classical algorithms of fractal dimension calculation. The maximum of fractal dimension is observed when moiré pattern is centrosymmetric. This indicates that rows lose some of individual subjects, and moiré bands are then formed on their total deformation field.

Defect structure of Mo/MoO/p-CdTe/MoO/Mo heterostructures according to high-resolution X-ray diffractometry

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Cadmium telluride (CdTe) is a semiconductor material with a wide range of applications. Due to the large band gap and high atomic number of metals that gives high quantum efficiency, CdTe-based detectors of X- and γ -radiation are widely used in such areas as space industry, medicine and more. [1]

X-ray studies were performed on a Panalytical Philips X'Pert PRO diffractometer for $CuK_{\alpha 1}$ radiation. The structures were fabricated by the deposition of MoOx films on the heated surface of CdTe substrates in a Leybold–Heraeus universal vacuum system L560 by means of the DC reactive magnetron sputtering of a pure molybdenum target (99.99% Mo) in the atmosphere of a mixture of argon and oxygen.

Structural perfection of studied samples was evaluated by the values of full width at half maximum of peak (W), maximum intensity (Ihmax), integral intensity (S), the peak shape of coherent scattering region, and also by analysis of the diffuse component (fig 1a).



Fig.1. Experimental distribution $I_h(\omega)$ (a) and Williamson-Hall plot for a series of symmetric (hhh) reflexes and evaluation of N_s in samples No1-No2 (b).

At the same time, the possible densities of screw dislocations were calculated using Williamson-Hall plot according to the value of mosaic blocks tilt angle α (fig 1.b).

The electrical and spectroscopic properties of the Mo/MoO/p-CdTe/MoO/Mo Schottky-diode heterostructures have been studied by the measurements of I-V characteristics and spectra of ²⁴¹Am and ¹³⁷Cs radioisotopes, respectively. The correlations between the crystal structure and the Mo/MoO/p-CdTe/MoO/Mo detector performance have been found.

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Theoretical background of metal-like films obtaining

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Intensive interest in development of new effective obtaining methods of coatings from metal-like refractory compounds (MLRC), particularly, from carbides, borides, and silicides of IV-VI group metals, is caused by their continuously extended field of application for contemporary industrial needs. Comparative analysis of existing methods of MLRC synthesis has shown that one of promising but poorly studied approaches is High-Temperature Electrochemical Synthesis (HTES) in ionic melts.

MLRC HTES is based on multielectron reactions of electroreduction of metals and non-metals from ionic melts. Principle of HTES method lies in formation of refractory compounds as a result of cathode or anode reactions. Common HTES parameters are as follows: at the temperature 100-1500 K, usually in air, during up to 2 h.

As molten electrolytes for HTES, molten refractory elements compounds, together with neutral (background) electrolytes with dissolved reagents, can be used. Using such electrolytes, all refractory compounds classes could be obtained. In such a case, one reaction component has to be electrode material (metal or non-metal). Gas electrodes are possible as cathodes. Obtained refractory compounds can be deposited onto electrodes as coatings, powders, or can go down to bath bottom as a sludge.

Interacting compounds can be dissolved in the background electrolyte both as neutral atoms or molecules and as charged ions or complexes. Such electrolysis type is primarily used for refractory compounds synthesis. As a result of cathode reactions, borides, carbides, silicides, and nitrides synthesis is possible, and as a result of anodic ones – only nitrides and oxides obtaining can be realized. Depending on synthesis components nature, there is a wide variety of possible HTES method realization ways.

During last 15 years, intensive studies of HTES theoretical background, multielectron processes realization and control principles, as well as their mechanisms, were carried out. Literature data analysis points out increased interest to IV-VI B group metals refractory compounds protective coatings electrodeposition from ionic melts. HTES of borides coatings is mainly developed as joint electroreduction of two electrolyte components for fluoride, fluoride-chloride, and fluoride-chloride-oxide melts. The main attention was paid to synthesis of titanium and zirconium borides, and to the less extent – of chromium and tantalum borides. HTES of carbides coatings is mainly developed for fluoride-carbonate, halide-oxide, and oxide melts. The main attention was paid to synthesis of molybdenum, tungsten, tantalum, and niobium carbides. HTES of silicide coatings is studied to the much less extent, and now its development is only at initial stages.
Inner size effect of the temperature coefficient of electrical resistance in film systems

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The temperature coefficient of electrical resistance (TCR) is an important characteristic of technological materials. It is TCR in many cases that determines the applied and physical properties of materials. In particular, information on the temperature dependence of the electrical resistance is needed to predict the functional characteristics of electronics components operating at elevated temperatures. The study of TCR of samples with metallic conductivity allows establishing the particularities scattering of electrons in the studied system. In addition, changes in the temperature dependence of the electrical resistance observed in vacuum condensates are used for studying supercooling, solubility, and diffusion in thin-film systems.

For today TCR is reliably determined for bulk metals samples. However, in the transition to nanostructured samples, the manifestation of the particularities of the temperature dependence of the electrical resistance should be expected. Moreover, in view of our previous studies (in particular devoted to the phenomenon of inner size effect of melting), the manifestation of particularities in the TCR can be expected even for vacuum condensates with a thickness of tens and hundreds of nanometres. The behavior particularities of such virtually massive objects can be explained by their internal nanostructure.

Our work is devoted to the study of the temperature dependence of the electrical resistance of Cu, Ag, V, and Mo films obtained by the method of vacuum condensation. Cu and Ag films were obtained using thermal, and V and Mo – electron-beam evaporation. The electrical resistance of the samples was measured by the standard four-probe method without letting air into the vacuum chamber.

It is established that the temperature coefficient of electrical resistance in Cu and Ag films in the thickness range of 20–100 nm is approximately constant. However, it turned out to be about three times smaller than the value known for bulk samples.

Along with this, the temperature dependence of the electrical resistance in films V and Mo is qualitatively different from the bulk samples. The resistance of these films decreases linearly with the temperature, which is completely untypical for metals. The established features of the temperature dependence of the electrical resistance were explained by the fine-dispersed nature of Cu, Ag, V films and the amorphous state of molybdenum samples.

Mo (W) – Ni (Co) intermetallides thin films: obtaining and properties

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The difference in the potentials of Ni and Mo deposition is 0.09-0.115 V at 1173 K in tungstate melt. A Na₂WO₄-2.5 mol % MoO₃ melt was used as an electrolyte to deposit alloys of various compositions. Mo thin films were electrodeposited using a molybdenum anode in the temperature range 1123-1173 K at a cathodic current density ranging from 0.02 to 0.15 A/cm². For the cathodic alloy co-deposition, the concentration of MoO₃ was maintained at 1.0-2.5 mol %, and the NiO – varied from 0.1 to 1.0 mol %. The molar ratio of Mo to Ni ions changed from 250 to 1. An increase in the NiO concentration or the temperature and a decrease in the cathodic current density increase the nickel content in the deposit. Continuous layers of MoNi, MoNi₃, and MoNi₄ intermetallics are sequentially deposited on the cathode at 1123-1173 K from the melts containing 0.1-1.0 mol % NiO. All of them have fine-grained or layered structure, and their microhardness H decreases in this series from 7.15 to 3.45 kN/mm².

The difference in the potentials of Ni and W deposition is 0.13-0.16 V at 1173 K. The starting melt was the Na₂WO₄–5.0 mol % WO₃ melt. In this case, the deposition dependences are similar to those obtained for the Mo-Ni alloys. The difference in the potentials of cobalt and tungsten deposition is 0.08-0.14 V at 1173 K. The Na₂WO₄-1.5 mol % WO₃ melt was used as an electrolyte for alloys thin films deposition. In this electrolyte, W coatings with a columnar structure form at current densities of 0.04-0.12 A/cm²: they are 0.2 mm thick and have a microhardness of 3.40-4.20 kN/mm². The experiments were carried out at cathodic current densities of 0.075-0.12 A/cm² in the temperature range from 1123 to 1173 K. The WO₃ concentration was maintained at 0.1-1.5 mol %, and that of CoO was changed from 0.01 to 1.0 mol %. The molar ratio of the W to Co ions was varied from 250 to 1. An increase in the CoO concentration, a rise in temperature, and a decrease in the cathodic current density increase the cobalt content in the deposit. Continuous layers of the CoW and Co₃W intermetallics thin films are sequentially deposited on the cathode at 1123-1173 K from the melts containing 0.1-1.0 mol % CoO. Their microhardnesses exceed those of the individual components of the alloys, being 8.40 and 5.00 kN/mm², respectively.

These dependences of electrodeposition of W-Co alloys are also characteristic of the deposition of Mo-Co alloys. Continuous deposits of Mo, CoMo, Co₃Mo, and Co thin films can be prepared from a Na_2WO_4 –MoO₃–NiO melt.

Evolution of the atomic composition and structure of the interfacial boundary in the aluminum-silicon system

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Aluminum layer can be used as the rear-side contact in commercial silicon wafer solar. Al and Si can intermix to form a phase segregated heterogeneous mixture, however Al and Si can also interdiffuse into each other in this process. Depending on the degree of interdiffusion, Al can act as a p-type dopant in Si, or a silicide can form. Both interdiffusion and heterogeneous mixing of Al+Si influence the optical response of this interfacial region. As a result of the mixing, the Al+Si interface at the rear of Si solar cells absorbs long wavelength photons not collected in the Si photovoltaic (PV) absorber; these long wavelength photons may be converted into heat and reduce operating device efficiency [1].

Aluminum has also been suggested as an improved candidate for UV plasmonics, one which benefits from chemical and thermal stability, low cost, and CMOS compatibility. Al nanohole arrays on silicon surface are thus attractive candidates for UV filter design [2].

Due to the great interest in the processes that occur during the interaction of aluminum and silicon, in our work the changes in the atomic composition and the transformation of the structure at their interface were investigated. The study was performed by the method of molecular dynamics using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package. The interaction between atoms was calculated using the Modified embedded atom method (MEAM) potential.

For the analysis of the atomic structure of aluminium-silicon interface depending on the temperature, a formalism of quasi 2D pair correlation functions (q2D-PCF) was used. Due to the fact that the system under investigations is partially liquid and partially crystalline, we have calculated the distribution of atomic density (density profile) and atomic content at the boundary of two phases in the direction perpendicular to the silicon surface.

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Magnetron plasma enhanced chemical vapor deposition (MPE-CVD) as novel and effective method for deposition of nanoporous a-C:H:N films for gas sensor applications

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It is reported a novel approach for the plasma enhanced deposition using planar magnetron discharge in low power/high pressure mode. In this mode the low discharge power and high pressure provide stable magnetron plasma discharge, however the flux of sputtered material from the cathode-target onto the substrate is negligible. Providing the substrate is located in the contact with plasma it is possible to realize the plasma enhanced deposition process using reactive gases. Specific feature of such process is low kinetic energy of the neutral and charged particles participated in deposition process, that promotes a formation of low-density material due to low surface mobility of the adatoms/radicals. Recently such process has been developed and applied for the deposition of low-density a-C:H films using methane and acetylene as reactive gas [1]. In the present research it is demonstrated a great potential of such method for the deposition of highly porous nitrogen doped amorphous hydrogenated carbon films (a-C:H:N). It is shown that nitrogen is readily incorporated in the carbon network in such processing and strongly effects on structure, photoluminescence and electrical properties. It has been found that incorporation of nitrogen strongly reduce film density by enhancing nanoscale porosity, and improve their electrical conductivity. High nanoscale porosity in combination with appropriate conductivity make these films highly attractive as a material for gas sensing systems.

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Nanosized levels of self-organized structures formation in gradient modified non-crystalline materials of Ge(As)-Te(S,Se) systems

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Gradient modified structures of As(Ge)-S(Te) systems are very interesting objects with wide practical and fundamental applications [1]. The fundamental researches using synergetics of the self-organizing processes and formation of self-organized structures in them, is extremely also important and unique [2].

The above-mentioned approaches are presented in this thesis. Having analyzed Fig.1 for the structure $\langle Ge_2S_3:Te \rangle$ (Te – 30,7 at.%) it is clear that the parameters characterizing the roughness value are significantly different from the previous results [1]. This difference in the values for structures with Te is explained by the presence of two halogens with different structural parameters in the film. That is resulting in the possible substitution of sulfur by tellurium and a partial disordering of an amorphous matrix frame on the basis of vitreous Ge₂S₃ (the height of the roughness reaches 37 nm).The formation of obtained condensates at given concentrations of solid solutions according to the mechanism of steam-solid phase with the implementation of a large number of large-sized islets are considered.



Fig.1. Axonometric image and sectional analysis of the gradient film surface $\langle Ge_2S_3:Te \rangle$ (Te – 30,7 at.%).

A significant emphasis is placed also on the study of self-organization processes of non-crystalline materials in the presence of external white noise [2]. The use of object-oriented modelling, which is de facto built on the principles of synergetics, is essential in the implementation of this approach.

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POSTER REPORTS Session 2 Nanotechnologies and nanomaterials, quantum-size structures



Electron beam induced effects in chalcogenide films

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The features of the interaction of the electron beam with chalcogenide films Ge_4Se_{96} and As_4Se_{96} have been studied. The films were irradiated by an electron beam from a Tescan scanning electron microscope, model VEGA. The primary electron energy was 30 keV, spot size 640 nm, electron beam current 60 nA. The surface relief of the films was scanned using a Bruker atomic force microscope, model ICON. The electron irradiation dose varied from $1.86*10^2 \mu$ C/cm² to $9.3*10^7 \mu$ C/cm² per point when a change in the irradiation time from 10 µs to 5 s.



Figure 1. AFM images and changes of the parameters of the electroninduced surface relief of Ge_4Se_{96} and As_4Se_{96} films depending on the irradiation time: height - the height of the cones, depth - the depth of the craters.

It was found that three types of surface relief are formed on the films surface when changing the irradiation dose in this interval. The change in the parameters and shape of the electronically induced surface relief for the Ge₄Se₉₆ and As₄Se₉₆ film is shown in Fig. 1. The irradiation sensitivity of Ge₄Se₉₆ film is $1.86*10^2 \ \mu\text{C/cm}^2$ (t₀ = 10 μ s) and of As₄Se₉₆ film is $6.51*10^2 \ \mu\text{C/cm}^2$ (t₀ = 35 μ s).

It is shown that the appearance of the surface relief is due to the formation of a space charge region in the volume of the locally irradiated film region. The dependence of the shape and parameters of the electron-induced relief is explained within the framework of the two-layer charge model. It assumes the presence and change in the shape of the surface relief depending on the magnitude of the electrostatic interaction in the space charge region.

Nanocrystallization of amorphous alloy Al₈₇Ni₈Dy₅ induced by heat treatment

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Strengthening of Al-based alloys is one of the main problems standing before researchers during long time. This problem exists not only for crystalline materials but also for amorphous ones, which reveal unique properties and are potentially useful for various areas of practical application. Most of widely used Al-based amorphous alloys consist of aluminum, transition metal (TM) and rare earth element (R) and reveal unique properties, first of all such as high specific strength, good ductility and good resistance to wear and corrosion. Certainly those main properties, which are responsible for application of these alloys, are related with structure features and their variation with temperature and concentration of constituent elements. On that reason the Al-based amorphous alloys attract interest of researchers in order to have a deeper understanding the nature of amorphous alloys and to know how features of atomic ordering are related with properties, most important for practical application.

Unfortunately, the current studies on relationship between such features of structure and kinetics of nanocrystalization of amorphous alloys at thermal annealing are poor.

On that reason the aim of this was to study the structural features of $Al_{87}Ni_8Dy_5$ amorphous alloy at different temperatures and the structural aspects of nanocrystallization. It is known that presence of nanoparticles in amorphous alloys promotes the significant improving of mechanical properties (ductility, strength, tensile fracture strength). Moreover early we have studied the structure and nanocrystalization features of amorphous alloys in Al-Ni-Y ternary system and it interesting how the substitution of Y by D-atoms will change the structure as well as nanocrystalization process.

On the basis of X-ray research it is established that at the first stage of primary crystallization (420-465K) there is a simultaneous nucleation and threedimensional growth of Al-nanocrystals. Within temperature range 465-580K the probability that new Al- nuclears are created significantly decreases due to that amorphous phase is enriched with Ni and Dy-atoms and consequently the diffusion controlled growth of Al-nanocrystals is the main contribution into kinetics of transformation.

About size-strain plot methods in diffractometric and modelling diffraction lines

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In order to determine the parameters of a nanostructure, the method of analyzing the width of diffraction lines is often used due to its simplicity. However, there is a need to make some comments about using integral width

In general, extensions occur both at the expense of physical factors (the presence of micro-strains and areas of coherent scattering), and instrumental (geometric) factors (beam divergence, focusing). If the instrumental factor is already taken into account, then extensions occur of physical factors is the presence of micro-strains and coherent scanning regions (CSR).

Mathematically, the extension of a line is described by a convolution operation. In the case of Cauchy functions, we get the sum of integral widths and in the case of Gauss function we get the sum of square of integral widths. Also, it should be noted that the ratio of the dimensions of the CSR determined using the integral width to the dimensions of the blocks determined from the width at half the height of the maximum of diffraction lines for the Cauchy function is equal to 0.71, and for the Gauss function -1.06.

In determining the size of the CSRs and the micro-strains values, the Williamson-Hall method is used to take into account the information from all diffraction peaks. The estimation of the above parameters also can be obtained by using a linear plot of size-strain plot methods (SSP) method. In this approximation, the reflex extension due to the particle size can be described using the Lorentz function, and the expansion of the reflex due to the micro-deformations of the crystal lattice – the Gaussian function.

In many publications (even with a significant number of citations), for the given method is written expression $(d_{hkl}\beta_{hkl}\cos\theta)^2 = \frac{K}{D}(d_{hkl}^2\beta_{hkl}\cos\theta) + (\varepsilon/2)^2$, which is faulty (in particular, the unit of measurement of each part of the expression is different). The correct formula looks like $(d_{hkl}\beta_{hkl}\cos\theta/\lambda)^2 = \frac{K}{D}(d_{hkl}^2\beta_{hkl}\cos\theta/\lambda) + (2\varepsilon)^2$. We can write the dependence $(d_{hkl}\beta_{hkl}\cos\theta/\lambda)^2$ of $(d_{hkl})^2\beta_{hkl}\cos\theta/\lambda$, which is approximated by the linear function y = A + Bx. In this case, the size of the CSRs is determined by the inclination of the approximating line, and the value of the micro-deformations is determined according to the formula $\varepsilon = 0.5\sqrt{A}$. Calculations using the right expression give results similar to the results of the Williamson-Hall method.

Thus, when comparing the sizes of crystallites obtained by different researchers, it is necessary to take into account methods by which they were determined. They must also be specified in the publications, or at least the name of the software that was used.

The crystalline structure of lanthanum-containing perovskite materials synthesized by sol-gel method

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The oxide compound $LaFe_{0.5}Cr_{0.5}O_3$ was synthesized by sol-gel method with the participation of auto-combustion. To monitor the crystalline structure at all stages of synthesis X-ray structural researches were carried out. The diffractogram of xerogel shows the absence of peroxide phases and the presence of one phase of ammonium nitrate (IV). This demonstrates that the formation of a perovskite structure occurs during the auto-combustion of this xerogel.



Fig. 1. Diffractogram (a) and TEM-image (b) of synthesized powder $LaFe_{0.5}Cr_{0.5}O_3$.

Analysis of the diffractogram of synthesized powders (fig. 1, a) showed that sample LaFe_{0.5}Cr_{0.5}O₃ has a space group of symmetry Pm-3m (Cubic Singonia) with the lattice constant a = 3,904 Å and the volume of the unit cell V = 59,5 Å³, X-Ray density of material $\rho = 6,724$ g/cm³. All reflexes present at diffractogram are identified, therefore, the synthesized material is single-phase. The average size of coherent scattering regions is 17 nm which is determined from the diffraction lines. According to the results of X-ray investigation of the synthesized material, it can be assumed that the particles, on average, consist of many regions of coherent scattering. Confirmation of the above is the image of synthesized powder LaFe_{0.5}Cr_{0.5}O₃ (fig. 1, b) received by a transmission electron microscope (TEM).

As a result, we can say that synthesized by a sol-gel method with the participation of auto-combustion sample has a structure of perovskite, is single-phase, with size of coherent scanning regions 15-20 nm and average-sized particles 40-60 nm.

Investigation of the surface plasmon-polaritons excitation efficiency on aluminium gratings

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Detailed studies of the efficiency of excitation of surface plasmonpolaritons (SPP) on aluminum gratings with a period a = 694 nm, which exceeds the incident wavelength of $\lambda = 632,8$ nm, have been carried out. The gratings relief depth (*h*) range was 6–135 nm. Для таких граток в досліджуваному інтервалі кутів падіння (0 – 90°) збуджуються два ППП, які відповідають +1 та -2 порядкам дифракції гратки, перший з яких вибрано в якості робочого.

Research samples were formed on $As_{40}S_{30}Se_{30}$ chalcogenide photoresist films using interference lithography and vacuum thermal deposition of an opaque aluminum layer about 80 nm thick. An atomic force microscope was used to determine the groove profile shape and the grating relief depth. The study of the SPP excitation features was carried out on a stand mounted on the basis of a G5M goniometer and an FS-5 Fedorov stage by measuring the angular dependences of the intensity of specularly reflected and diffracted *p*-polarized radiation of He-Ne laser. When determining the SPP excitation efficiency, the resonance values of both specular reflection and reflection in the -1st diffraction order were taken into account.

It was found that the dependence of the integral plasmon absorption on the grating modulation depth (h/a) is described by a somewhat asymmetric curve with a wide maximum, the position of which corresponds to an h/a value of about 0.07 and a half-width of about 0.123. This allows to excite SPP with an efficiency $\geq 80\%$ of the maximum value on the gratings with the 0,05-0,105 h/arange. The half-width of the plasmon minimum of the reflection in the -1st DO is less than in the specular reflection, which can increase sensitivity of sensor devices when registering the shift of the minimum from angular measurements. The dependence of the half-width of the SPP reflection minima on the grating modulation depth is close to quadratic. In the investigated h/a range (from 0.009 to 0.194), the maximum dynamic range of the reflection coefficient is two orders of magnitude and is achieved in specular reflection for gratings with $h/a \approx 0.075$.

Physic-chemical properties of nanocomposites by polymethacrylic acid and polyaniline

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Polymer-polymer composite (PPC) based on polymethacrylic acid (PMAA) and polyaniline (PANI) have electrical conductivity and have film-forming properties. Such PPCs can be successfully used to construct sensory devices. Composites were obtained by a mechanic-chemical method, mixing the calculated amounts of PMAA and PANI in a small amount of water. The resulting mixture was treated with ultrasound for 30 minutes, and swings were dried in vacuum for 48 hours.

Investigation of electrical conductivity of composites showed that at a content of ~10% weight PANI begins a sharp increase in electrical conductivity, which at 70% weight of conductive component reaches the values of a pure polymer. Morphological studies of composites indicate that at 10% weight of content PANI in PMAA matrix begins to form conductive chains. The study of the temperature dependence of the electrical conductivity indicates that the PPC has a semiconductor nature and is characterized by energy of activation of charge transfer of 0.51 ± 0.05 eV.

X-ray study of source polymers and PPC indicates the interaction between PMAA and PANI macromolecules. Quantum-chemical calculations have shown that macromolecules are strongly polarized, which promotes the formation of a strong intermolecular interaction. In addition, macromolecules can have different conformational states.

The quantum-chemical calculations of the thermodynamic parameters of PMAA, PANI and PPC indicate that hydrogen bonds between macromolecules that are part of the composite may be formed. The energy of intermolecular hydrogen bonds is calculated.

Solid state dewetting application in formation of In/InTe nanosystems

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The solid state dewetting method (SSD) as a promising way to obtain nanostructures has been extensively investigated in the past decades. Due the intrinsic bulk anisotropy of the InTe, a fresh (001) surface is easily obtained by cleavage even in UHV which makes it suitable as a template for obtaining nanosystems with reduced dimension with application of the SSD in situ. From a physical point of view effective pattern assembly requires nanostructure precursor's mobility over the substrate, a property that is naturally connected with layered crystal surfaces. In consequence of our studies it should be noted that the SSD method application combined with natural patterned surface topography of 2D layered crystals and their surfaces' poor adhesion are one among most perspective routes to self-assembling of metal nanostructures in producing arrays of nanoscale shapes for electronic and photonic devices and for catalyzing growth of nanodots, nanotubes and nanowires.

The formation of indium induced nanostructures on the (001) surface of scanning tunneling lavered semiconductor InTe was studied by the microscopy/spectroscopy (STM/STS) in UHV, as a function of indium coverage. The phase-elemental composition and structural perfection of InTe initial surface were characterised by X-ray photoelectron spectroscopy, low energy electron diffraction and atomic force microscopy. X-ray diffraction studies revealed InTe tetragonal crystal structure of the TlSe type (I4/mcm space group, lattice parameters a = 8.4414(6) Å, c = 7.1333(5) Å). Thermal evaporator EFM-3 was applied for In deposition in UHV. STM studies of initial (001) InTe surface with ~8 Å parameter square lattice subsequently used as an ordered template in SSD process show that the shape and arrangement of indium induced nanostructures are powered by this lattice symmetry as derived from tetragonal InTe bulk one.

The Omicron NanoTechnology STM/AFM System has been exploited in current imaging tunneling spectroscopy (CITS) mode to study the local distribution of density of states (LDOS) on the InTe cleavage. We observed the formation of nanosized 0D metallic structures in a result of the SSD process due to surface heating above the indium melting point. The STS reveal direct correlation between indium coverage kinetics and increase in the quantity of DOS at the surface within the band gap of InTe.

Quantum size effect in silicon nanowires

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Films of silicon nanowires have found application in solar energy, as broadband antireflection coatings in solar cells, and are also used for the manufacture of LEDs and chemical sensors.

The paper presents the results of a study of the optical reflection and transmission spectra of a silicon single crystal p-Si (100) with silicon nanowires grown on both sides and porous silicon p-Si (100) on a single crystal substrate in the spectral range $0.2 \div 1.7 \,\mu\text{m}$. The layers of nanowires had a thickness of 5.5 μ m, 20 μ m, 50 μ m and a porosity of 60 %. The porous silicon layers had a thickness of 5 μ m, 50 μ m and a porosity of 45 %, 55 % and 65 %. The change in the energy band structure in single-crystal silicon nanowires and in a single-crystal matrix of porous silicon is shown.

The energy of a quantum mechanical particle is described by the formula:

$$E(\mathbf{k}) = E_0(\mathbf{k}) + \Delta E(\mathbf{k}),$$

where k is the wave vector, $E_0(k)$ is the energy of the fundamental optical transition of the material under study; $\Delta E(k)$ is a quantum-sized addition to the hole energy (size quantization energy). The energy of the ground state increases or decreases by the value:

$$\Delta E = \frac{\hbar^2 \pi^2}{2m^* L^2} \,,$$

where m^* is the effective mass of a free particle, the motion of which is limited by infinitely high non-penetrating barriers located at a distance *L*.

According to experimental data and calculations, the decrease in the band gap of porous silicon p-Si (100) and silicon nanowires, in comparison with single crystal p-Si (100), is explained by the quantum size effect that occurs in the objects under study. It is shown that the energy spectra of the investigated structures depend on their specific surface area.

The absorption spectra of silicon nanowires are constructed and analyzed. The energy broadening ΔE of the optical spectra and the energy relaxation time of photogenerated charge carriers τ of the materials under study are estimated.

When writing this work, sources were used [1-3].

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Study of adsorption properties of graphene-like InP

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The semiconductor compounds in a state of graphene-like structure are the interesting object for both fundamental studies and technology. The twodimensional material have unique electronic, structural, chemical and physical properties that plays a significant role for technology of new devices. Therefore the obtaining of various properties of that graphene-like materials and the understanding of the nature of chemical interaction with various species are important. In this work the GAMESS program package [1] have been used.

Such species as hydrogen, oxygen and carbon are a part of many natural compositions of the environment. In this work the preferred adsorption sites for the H, O and C adatoms have been defined through the potential-energy profiles of its interacting with g-InP sheet.

All ab initio calculations reported in this work were carried out using the Hartree-Fock method of GAMESS program package. The GAMESS was run on computers cluster of V.M.Glushkov Institute of Cybernetics of NAS of Ukraine [2]. Both STO-3G and 3-21G Pople style basis sets were used for C, H and O atoms. The g-InP sheet has been presented by cluster model with 48 In-atoms and 48 P-atoms in the hexagonal cells and 24 hydrogen atoms on the cluster perimeter. In the atomic-force probe technique the atom-probe (H, O or C) is moving above the surface of sheet on fixed distance without any optimization of its geometry.



Fig.1. The scheme of moving of adatoms for computer simulation of surface diffusion.

As a result the potential-energy (PE) profiles of interaction of the various atoms-probe with g-InP sheet have been obtained. The determined mechanisms of interactions will be discussed.

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Structure, morphology and magnetic properties of NiFe₂O₄/rGO nanocomposites synthesized by self-combustion method

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Electrochemical performance, catalytic properties and electromagnetic interference shielding characteristics of ultrafine ferrites expand their scope of application by the use of composite materials with ultrafine carbon. NiFe₂O₄ / reduced graphene oxide (rGO) composites have been synthesized by solution combustion method using glycine as a fuel agent (the molar ratio of Ni : glycine was 1:1). GO has been prepared by the modified Hummers' method. Both pure ferrite (sample T0) and NiFe₂O₄/rGO composites (mass ratio of spinel and rGO phases was 3:1 (sample T1) and 3:2 (sample T2), respectively) have been obtained. Thermal reduction of GO has been carried out by self-propagating autocombustion. The influence of the amount of the rGO component and additional thermal treatment on the phase composition, size of oxide particles, and magnetic properties have been characterized by XRD, low-temperature nitrogen adsorption method, Mössbauer and impedance spectroscopy. Ferrite powders with a single spinel structure have been observed for all samples, when the halo in the XRD patterns of the composite powder observed at $2\theta=15-27^{\circ}$ corresponds to the (002) reflex of disordered rGO. An increase in the rGO content causes a decrease in the particle size from 15-18 nm for sample T0 to about 10-11 and 6-8 nm for samples T1 and T2, respectively, while reducing the degree of inversion of $(Ni^{2+}_{1-x}Fe^{3+}_{x})[Ni^{2+}_{x}Fe^{3+}_{2-x}]O_4$ mixed spinel. The Mössbauer spectra of sample T1 consist of a central doublet and a broadened sextet, which corresponds to the presence of both ferromagnetic and superparamagnetic ferrite particles, when the spectra for sample T2 indicate the transition of all particles to a single domain superparamagnetic state. The BET isotherms of composite samples correspond to type IV adsorption with a predominance of mesopores. The specific surface areas of samples T0, T1 and T2 were 28, 125 and 152 m²/g, respectively. The AC conductivity of asprepared and annealed samples has been analyzed using the Johnscher or Drude models. The presence of GO in the reaction medium affects the change in the size and morphology of particles during annealing in the temperature range of 200-800°C. Obviously, the GO component acts as a coolant, which leads to a decrease in the combustion reaction temperature, prevents particles from sintering, while additional gas evaporation during the reduction procedure hinders the formation of agglomerates. The results of the study make it possible to develop conditions for the synthesis of the NiFe₂O₄/ rGO nanocomposite with tuned properties, which are important for energy storage applications.

Effect of graphene oxide on the gas sensitivity of poly(3,4-ethylenedioxythiophene) films

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Over the years intensive research of low-dimensional materials with new useful physical properties and the production of gas sensors based on its are carried out [1–3]. The unique structure of poly(3,4-ethylenedioxythiophene) (PEDOT) determines its high conductivity, physical and chemical stability, biocompatibility and transparency in the doped state [4]. In order to test PEDOT thin films as potential sensitive elements of optical gas sensors, the influence of doping with graphene oxide (GO) nanoparticles on the conditions of obtaining, morphology and optical properties of PEDOT was studied.

PEDOT/GO films on SnO_2 were obtained by electrochemical deposition. According to TEM, the modification of PEDOT by GO nanoparticles causes an increase of the size of the structural globules from 80 to 250 nm while an increase of the sensory sensitivity of polymer films (10 times) to the action of NO_2 . In addition, due to the interaction of gas molecules with the sensory medium, the color of the PEDOT/GO film changes from dark brown to gray-violet. The optical response of hybrid sensory films is quite fast – 1-2 minutes.

As a consequence of the action of hydrogen sulfide vapors, there is an increase in the optical absorption of PEDOT/GO sensor films in the entire range. Moreover, the greatest changes are observed after 90 s of exposure. The contrast of optical transitions, calculated at $\lambda = 510$ nm, is ~ 91 % under the action of gas for 2 min, and for a longer duration it almost does not change.

The action of dymethylformamide (DMF) vapors causes significant changes in the morphology of PEDOT and an increase in the intensity of the π - π^* band transition at $\lambda = 490-500$ nm. At the same time, toluene vapors have practically no effect on the optical absorption of the PEDOT/GO films.

The revealed effect can be the basis for the selective detection of vapors various natures in industry and the environment, as well as in the design of optical sensors to control harmful emissions into the atmosphere.

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Porous structure of carbon materials obtained from the shell of walnuts

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The aim of this work is to study the effect of carbonization temperature of raw materials of plant origin (walnut shells) on the porous structure of the obtained carbon materials (CM). The carbonization process was carried out in the temperature range of 400 °C \div 1000 °C in steps of 100 °C.

To study the porous structure of the obtained porous CM used the method of small-angle X-ray scattering (SAXS). SAXS spectra were measured on an automated diffractometer DRON-3 equipped with three-slit collimators of primary and scattered radiation. The distribution functions of the effective pore radii were determined by the indirect Fourier transform method of the integral equation [1].

The volume distribution functions of the pores are shown in Fig. 1, illustrate significant changes in the distribution of porous space, which correlate with changes in the fractal characteristics of CM samples. The fractal dimension of the surface and there increases are significant changes in the pore volume distribution of the porous CMs samples with increasing carbonation



Fig. 1. Volumetric pore distribution functions

temperature of the source, which is especially evident for the sample obtained at 700 °C. As can be seen from Fig. 1, the most significant changes in the pore distribution are observed in the samples obtained at temperatures above 700 °C. It is shown that porous CMs obtained at 400-700 °C are macroporous materials, the maximum of the porous volume of which corresponds to pores with radius $R \approx 30$ nm, and samples obtained at 700-1000 °C are mesoporous with $R \approx 5$ nm.

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Photoconductivity of macroporous silicon in conditions of strong surface light absorption

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The surface photoconductivity in the structures of macroporous and single-crystal silicon was studied with an absorption coefficient in the range of $200 - 10^4$ cm⁻¹. In this case, positive and negative photoconductivity was observed. The starting material for the formation of macroporous silicon structures was n-type silicon with a [100] orientation and a resistivity of 4.5 Ω cm. Using electrochemical etching, macropores with a diameter of $D_p = 2 \mu m$, a depth of hp = 60 μ m and a period of a = 4 μ m were formed. It was found that when light is absorbed with a wavelength of 0.52 µm, a "slow" negative photoconductivity is observed at a thickness of the space charge region of 1 µm. When light is absorbed with a wavelength of 0.935 and 0.62 µm at a depth of 50 and 2.5 µm, respectively, positive photoconductivity is observed. The reason for negative photoconductivity is sticking at the "slow" surface levels of the main charge carriers; positive surface photoconductivity is manifested when sticking to minority charge carriers. Based on the measured negative photoconductivity, the photoconductivity of the inversion layer was calculated and from it the estimated concentration of "slow" surface levels was obtained both in the structure of macroporous (N> 10^{13} cm⁻²) and in single-crystal silicon $(N < 10^{13} \text{ cm}^{-2})$. It was shown that the ratio of negative photoconductivity values in the structure of macroporous silicon and in single-crystal silicon practically coincides with the ratio of the illuminated areas of the macroporous structure (taking into account the surface area of the macropores) and single-crystal silicon (27 and 25, respectively), which confirms the purely surface nature of negative photoconductivity under conditions of strong surface absorption of light.

It was established that when light is absorbed with a wavelength of 0.52 μ m, a slow negative photoconductivity is observed at a thickness of the space charge region of 1 μ m. When light is absorbed with a wavelength of 0.935 and 0.62 μ m at a depth of 50 and 2.5 μ m, respectively, a positive AF is observed. The reason for the negative phase transition is adherence at the surface levels of the main charge carriers; a positive surface phase transition appears when the minor carriers adhere.

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Photoconductivity Relaxation in the Macroporous Silicon in the Ultraviolet Range

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The "slow" relaxation of negative monopolar photoconductivity in the structures of macroporous silicon in the ultraviolet wavelength range of 360 - 410 nm was studied. Two relaxation times have been established, arising due to "slow" surface states localized at the Si / SiO₂ interface and in the SiO₂ dioxide layer, equal to 2s and 300 s, respectively. It was shown that of the three components of photoconductivity: bipolar photoconductivity σ_{b1} , monopolar photoconductivity σ_{m1} and bipolar photoconductivity quasineutral volume σ_{b2} under conditions of strong surface absorption, surface monopolar negative photoconductivity σ_{m1} dominates and determines the negative sign of the photoconductivity of the structure of macroporous silicon.



Fig. Dependence of normalized negative photoconductivity on relaxation time

The magnitude of the surface monopolar negative photoconductivity of macroporous silicon and its relaxation time depends on the light intensity. With an increase in the illumination intensity, the magnitude of the surface monopolar negative photoconductivity increased. This is explained by an increase in the adhesion of the main charge carriers at slow surface levels localized within 1 nm from the surface of the semiconductor in the transition layer SiO_x and in silicon dioxide SiO₂. The relaxation time decreased with an increase in the illumination intensity due to an increase in the surface bending zones.

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Polarizability of metal islands in the form of a truncated sphere on a dielectric substrate

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Hemispherical islands are obtained by the method of reverse diffusion. For such islands, the frequency dependence of the polarizability was studied in [1]. In [2] was demonstrated that thermal evaporation of a homogeneous metal film produces islands in the form of a truncated sphere, and the truncation angle depends both on the thickness of the initial film and on the annealing temperature. The relation for the dimensionless dipole polarizability (the case of an electromagnetic wave incidence normal to the surface of the dielectric substrate) of a metal island in the form of a truncated sphere, obtained from the solution of the corresponding electrostatic problem, has the form

$$\alpha_{\perp}(\omega) = \frac{12T_{m}\overline{\alpha}_{sph}}{4 - \overline{\alpha}_{sph} \frac{T_{d} - T_{m}}{T_{d} + T_{m}}},$$
(1)

where T_d and T_m are the dielectric constants of the substrate and the environment;

$$\overline{\alpha}_{\rm sph} = \frac{T(\omega) - T_{\rm m}}{T(\omega) + 2T_{\rm m}},\tag{2}$$

is a dipole polarizability of a spherical nanoparticle;

$$T(\omega) = T^{\infty} + \frac{\omega_p^2}{\omega(\omega + i\gamma)}, \qquad (3)$$

is a dielectric Drude function of the truncated sphere material; ω_p is the frequency of bulk plasmons; γ is the relaxation rate; τ^{∞} is the contribution of the crystal lattice to the dielectric function.

It follows from formula (1) that the polarizability of a truncated sphere differs significantly from the polarizability of a spherical nanoparticle. In addition, the shift of the polarizability maximum corresponding to the localized surface plasmon resonance will also be significant in this case.

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Electrochemical synthesis of nanopowders of chromium, molybdenum, and tungsten silicides and borides powders from halide-oxide melts

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Thermodynamics analysis and voltammetric studies have shown that High-Temperature Electrochemical Synthesis (HTES) of VI-B group metals silicides and borides is possible to realize only in kinetic mode. In such a case, stages sequence is the following: deposition of electropositive component (Mo and W as metal, Cr as oxide Cr_2O_3), deposition of second component (silicon or boron) onto surface of oxide or metal deposited before, diffusion of silicon or boron into depth of metal-salt bulb with formation of different silicide and boride phases up to higher silicides MSi₂ and borides MB₄.

HTES was carried out in molten KCl-KF-K₂SiF₆-K₂CrO₄ mixtures. Depending on electrolyte composition and parameters of electrolysis, both individual phases (Cr_2O_3 , Cr_3Si , and $CrSi_2$) and their mixtures with low content of silicon were obtained.

Electrosynthesis of molybdenum and tungsten silicides nanopowders was carried out in molten NaCl-Na₃AlF₆-Na₂MO₄-SiO₂ mixture (where M-Mo, W). At the temperature below 1123 K, Mo (W) and Si reaction completeness is not reached. With temperature higher than 1223 K, metal-salt bulb stability lowers, and silicides have not formed. With optimal melt composition, pure double silicides MoSi₂ and WSi₂ are formed at i_k =0.5-1.2 for MoSi₂ and 0.5-1.5 A·cm⁻² for WSi₂. Specific surface area of powders was 5-15 m²·g⁻¹, particles size was 0.5-2.0 µm.

Electrochemical synthesis of chromium borides nanopowders was carried out from molten mixture of NaCl-Na₃AlF₆-K₂CrO₄-B₂O₃. Depending on melt composition and electrolysis parameters, both individual Cr₂O₃, Cr₂B, CrB, and CrB₄ phases and their mixtures were formed. Powders specific surface area is 8-17 m²g⁻¹.

Electrochemical synthesis of molybdenum and tungsten borides nanopowders was carried out in molten NaCl-Na₃AlF₆-Na₂MO₄(MO₃)-B₂O₃(Na₂B₄O₇) mixture. Optimal concentrations of MO₃ or Na₂MO₄ were 0.75-1.5 % (w/w). With higher concentrations, due to instability of metal-salt bulb, complete boriding of deposited refractory metal is not achieved. Within the interval of B₂O₃ and Na₂B₄O₇ concentrations 10-20 % (w/w), complete boriding of refractory metal takes place, and MoB₄ or WB₄ phase is obtained. Specific surface area values for MoB₄ and WB₄ powders were 5-15 m²·g⁻¹.

Mechanisms of scattering of current carriers in polycrystalline PbTe films

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Lead telluride films are promising materials for detectors and sources of infrared radiation. Carrier scattering mechanisms have an important effect on the performance characteristics of device structures based on them.

The dependence of the mechanisms of scattering of current carriers in thin polycrystalline PbTe films on the thickness of $2.5-7.7 \mu m$ was studied in the temperature range 77-300 K.

Films for the study were obtained from the vapor phase by the hot wall method on glass substrates. The growth rate of the films was 1-3 NMS-1. The structure of the films was studied by electron microscopy and diffraction, as well as optical metallography. Measurements of the electrical parameters of the films were performed by the compensation method in constant electric and magnetic fields. Measurements were performed on individual films of different thickness. The current through the samples was about 0.1 mA. The magnetic field had a direction perpendicular to the surface of the films at an induction of 0.8 T. The measured sample had four Hall and two current contacts.

The films were polycrystalline with crystallite sizes of about 1 μ m, which were clearly formed lamellar structures oriented mainly by the {100} planes parallel to the surface of the glass substrate with a significant orientation in azimuth.

For these films, the value of n = 0.7-1.4 was obtained. Thus, for the studied film thicknesses, the index n of the temperature dependence of the mobility confirms the dominance of charge carrier scattering at the intergrain boundaries. It should be noted that the thickness dependences of the mobility of the current carriers of PbTe films, calculated under the condition of scattering at intergrain boundaries, differ slightly from the experimental ones..

The activation energy of electrical conductivity, calculated from the temperature dependence of Hall mobility, is 0.04-0.07 eV [1]. It is proved that the activation energy is associated with scattering at intergrain boundaries.

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Thickness oscillations of the Seebeck coefficient in (Bi_{0.9} Sb_{0.1})₂Te₃ topological insulator thin films

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The Bi_2Te_3 semiconductor compound and $(Bi_{1-x}Sb_x)_2Te_3$ solid solutions are presently among the best low temperature thermoelectric materials which are extensively used in manufacturing refrigerating devices. Recently, interest in the transport properties of these materials has grown sharply due to the observation of the topological insulator properties in their crystals and thin films. Electron confinement in low-dimensional structures leads to a radical change in the physical properties of these materials as compared with bulk crystals and provides new ways for controlling thermoelectric properties of solids.

Earlier, in thin polycrystalline films of p- and n- Bi₂Te₃, we observed thickness oscillations of transport coefficients [1,2] and attributed them to the manifestation of size quantization of the energy spectrum. It is of interest to find out how the cation substitution in Bi₂Te₃ will affect the manifestation of size quantization in thin films with sufficiently small thicknesses.

The goal of the present work is to study the room temperature dependences of the Seebeck coefficient on the thickness of $(Bi_{0.9} Sb_{0.1})_2Te_3$ polycrystalline thin films grown on glass substrates with a view to observing the quantum oscillations.

The dependences of the Seebeck coefficient on the thickness (d = 15-100 nm) of the thin films grown on glass substrates by thermal evaporation in vacuum of the *p*-type (Bi_{0.9} Sb_{0.1})₂Te₃ topological insulator polycrystals were measured at room temperature. It was established that these dependences exhibit an oscillatory behavior. The possibility of the observation of such oscillations in a polycrystalline film grown on an amorphous substrate is explained by the presence of texture in the (Bi_{1-x}Sb_x)₂Te₃ thin films in the electron confinement direction. The obtained results are interpreted in terms of quantum size effects. The oscillation period Δd calculated theoretically within the framework of the simplest idealized model of a rectangular potential well with infinitely high specularly reflecting, smooth, and identical walls is in good agreement with the experimental data.

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Effective carrier lifetime in two-sided macroporous silicon as a function of the bulk lifetime

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One and two-sided macroporous silicon is used to create chemical sensors, sensors, photodetectors and solar cells. An important characteristic of these devices is the effective lifetime of charge carriers, which we consider in two-sided macroporous silicon [1]. The paper considers the analytical derivation of a system of two transcendental equations, the numerical solution of which is the effective lifetime of minority charge carriers in two-sided macroporous silicon. For the analytical derivation of the system of two equations, we used the general solution of the diffusion equation written for each macroporous layer and a single-crystal substrate between them. We supplemented the general solution with boundary conditions written for the boundaries of a single-crystal substrate with macroporous layers and sample surfaces.



Fig. The normalized effective lifetime of minority charge carriers in two-sided macroporous silicon as a function of the bulk lifetime and pore depth.

It is revealed that the effective lifetime in two-sided macroporous silicon depends on the bulk lifetime, the rate of surface recombination, the thickness of the single-crystal substrate, and the geometric characteristics of the pores of each macroporous layer, such as: the average pore diameter, the average distance between the centers of the pores, and the average pore thickness.

It is shown that the effective lifetime is limited by the diffusion of charge carriers from the substrate to each macroporous layer if the rate of surface recombination in the macroporous layers is too high.

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Distribution of excess charge carriers in bilateral structures of macroporous silicon with nanocoatings for solar cells

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A solar cell structured on both sides absorbs not only incident but also reflected light [1], therefore, it is urgent to study the distribution of excess charge carriers in bilateral macroporous silicon with nanocoatings for solar cells. Due to the presence of macropores and coating on the surface, reflections are reduced and light absorption is improved. The bilateral structures of macroporous silicon improve the absorption of light by the front and back surfaces, reflecting it between surfaces and increasing the optical path through light scattering. The distribution of excess charge carriers is found from the diffusion equation. The diffusion equation was written for two layers of macropores and a substrate and supplemented with boundary conditions.



Fig. Stationary distribution of the normalized concentration of excess minority charge carriers in double-sided macroporous silicon over the sample thickness for the wavelength spectrum, μ m: a) 0.55-0.8, b) 1-1.05.

It is revealed that in the visible spectral region the distribution of excess charge carriers in double-sided macroporous silicon has two maxima, which are caused by the illumination of the sample and the bottom of the pores, as well as an exponential decay. In the near-IR region of the spectrum, the distribution of excess charge carriers in double-sided macroporous silicon is symmetric with respect to the middle of the sample and has one maximum due to weak absorption of light from this region of the spectrum.

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Effect of Gas Adsorption on the Photoluminescence of Doped Zinc Oxide Nanopowders

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The study of the photoluminescence features in different gas environment (vacuum, air, O_2 , N_2 , H_2 , CO, CO₂) of ZnO:Ni (Cd) nanopowders obtained by pulsed laser reactive technology [1] has been carried out. Structural, optical and luminescent properties of the nanopowders were studied by X-ray diffractometry, electron microscopy, transmission and photoluminescent spectroscopy. Nanopowders have high optical transmission in the visible and near-IR regions of the spectrum. Fig.1 shows the room temperature photoluminescent spectra of ZnO:Ni with excitation wavelength at 365 nm. The

peculiarities of the influence of surface doping by impurities (Ni, Cd) on the sensitivity and selectivity of the signal response during adsorption of established. gases are The decomposition of luminescence spectra into elementary bands shows the presence of four elementary peaks. The most intense two bands in visible region which are sensitive to ambient blue-band gas, a centered at 430 nm and



Fig.1. Photoluminescent spectra in different gas environment of ZnO:Ni nanopowder

stronger in intensity the band around 520 nm. The character of visible photoluminescence determined by the intrinsic defect structure of the material and depends on the technological parameters obtaining of nanopowders. Changing the ambient leads to a significant change in the intensity of the photoluminescence spectra and its deformation. Obviously, this is a result of the redistribution of existing luminescence centers and the emergence of new luminescence adsorption centers on the nanopowders surface. The investigated nanopowders can be effectively used as sensitive materials for the construction of gas sensor systems

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Effect of various capping agents on optical properties and stability of MnS nanoparticles

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Nanostructured MnS ($E_g \ge 3.7 \text{ eV}$) have attracted great interest in many application fields including solar cells, fuel cells, light-emitting diodes, solar cells sensors, supercapacitors, Li-ion batteries, semiconductor photocatalysts, and thermoelectric devices [1].

Relatively small list of stabilizers are known as a capping agent for the MnS NPs synthesis. Thus, the objective of this paper is to study perculiarities of formation of MnS NPs capped by various stabilizers in aqua solvent at room temperature. To compare a stabilizing effect on the MnS NPs of two thiols, namely, L-cysteine (L-cys) and thioglicolic acid (TGA) with citrate-ions the syntheses were provided at the same conditions (equal content of the precursors and coordination number (c.n.) for the ligands).

Manganese chloride tetrahydrate $MnCl_2*4H_2O$, L-cysteine $HO_2CCH(NH_2)CH_2SH$ (L-cys), thioglycolic acid HS-CH₂COOH (TGA), Trisodium citrate dihydrate $C_6H_5Na_3O_7*2H_2O$ and Sodium sulfide Na_2S*9H_2O (Sigma Aldrich) were used unaltered for the synthesis.

Two stock aqua solutions of 0.005M (Seria A) or 0.05 M (Seria B) $MnCl_2*4H_2O$ were used as precursors for the Mn/ligand complexation. While the solutions of Seria A were characterized by $[Mn^{2+}]:[S^{2-}] = 1:1$ and 1:2 and the ligands coordination number c. n. = 2; 4 and 6, the solutions of Seria B contained double excess of the anion at c.n. = 2 only. In each Series of experiments, both collections of data are processed simultaneously.

The optical properties of the ligands and their complexes with manganeseions stock solutions as well as stability of as-prepared MnS particles were studied by monitoring the UV–vis absorbance and photoluminescence spectra. The results indicate that the capping agents effectively stabilized MnS NPs only at relatively small the precursors content (including their quantity in Series A of the experiments). Higher in order concentration of the precursors had resulted in rapid growth of the products' sizes and their precipitation demonstrating diminishes of the stabilizing action.

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Optical-Luminescence Properties of ZnO and TiO₂ Nanopowders, Obtained by Pulsed Laser Reactive Ablation

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ZnO and TiO₂ nanopowders were prepared by means of the pulsed laser reactive ablation of metallic target (Zn, Ti). Structural, optical and luminescent properties of the powders were studied by X-ray diffractometry, electron microscopy, transmission, Raman and photoluminescent spectroscopy. X-ray diffraction studies have shown that ZnO samples have a crystalline structure of wurtzite and TiO₂ samples have a crystalline structure of rutile. Peaks that may correspond to impurities were not detected, which indicates the high purity of the obtained materials. All samples have high optical transmission in the visible and near-IR regions of the spectrum. Fig.1 shows Raman scattering spectra of initial and laser annealing ZnO and TiO₂ nanopowders. Based on the phonon mode analysis in the Raman spectrum nanopowders the character of the quality of the crystal structure are determined and their evolution in the process of laser annealing.



Fig.1. Raman scattering spectra of initial (1) and laser annealing (τ =10 ns, n=28 Hz, E=0.1 J/cm²) during 10 min (2), 20 min (3), 40 min (4) ZnO (a) and TiO₂ (b) nanopowders.

It was found that pulsed laser annealing makes it possible to significantly modify the luminescent properties of nanopowders by changing its intrinsic defective structure. The dependence of the photoluminescent intensity of nanopowders on the excitation wavelength has been studied, and the optimal wavelengths to excitation the luminescence were established.

Metallothermic obtaining of chromium disilicide nanopowders technological processes of, molybdenum and tungsten synthesis by reduction method

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To obtain chromium disilicide nanopowders by metallothermic synthesis method, 0.02 mol of completely dry chromium trichloride and 0.04 mol of sodium fluorosilicate were placed into quartz container. After 0.22 mol potassium metal have been added, the container was put into the reactor made of stainless steel, and argon atmosphere was created. The reactor was heated up to 650-750 ^oC and leaved for 10-15 hours.

Metallothermic reduction process can be presented as follows. At temperature higher than 450° C, sodium fluorosilicaste decomposes to NaF and gaseous SiF₄. Probably, chromium disilicide synthesis reaction is based on interaction between chromium and silicon formed through chromium (III) chloride and silicon (IV) fluoride reduction by metallic potassium.

Compounds NaF, KF and KCl formed during synthesis are by-products. Melting temperature of salt system based on these compounds is $600-650^{\circ}$ C. Since reaction temperature is higher than melting temperature of salt mixture, reaction between Cr and Si with CrSi₂ formation can be realized in molten fluoride-chloride system. Molten phase favours nanocrystalline product formation.

All peaks at powders X-ray patterns can be attributed to chromium disilicide hexagon phase. Results of synthesized powders structural study provide evidence that they consist of nanoparticles. Average size of chromium disilicide particles is 35-60 nm.

Thermostability of synthesized powders in air flow at temperatures up to $1000^{\circ}C$ determined thermogravimetric by and differential was thermogravimetric analysis methods. According to data of thermogravimetric analysis, mass of synthesized dicilicide powders is practically stable up to 700 ⁰C. Unsignificant mass changes are connected with losses of water adsorbed on powders surface. Quantity of adsorbed water is very small, and that is why it is impossible to find endothermic peak at the differential thermal analysis curve at corresponding temperature. Within temperature range from 700 up to 1000°C, synthesized powders mass increases gradually up to 7.4%. At differential thermal analysis curves, one significant exothermic peak is observed within the temperature range 815-820°C. Correlation of gravimetric and thermogravimetric curves allows one to assume that synthesized powders do not oxidize at temperatures up to 700°C. During further temperature increasing, significant oxidizing is occurred at powders surface. This process became more intensive at temperatures 815-820°C. As a result, protective oxide layer is formed at the powders surface.

Synthesis of «porous silicon – cadmium telluride» nanocomposites and study of their properties

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Currently, there is great interest in composite systems, which consist of a matrix and embedded in the matrix of materials or nanoobjects. The interest is due to the fact that the control of the physical properties of such systems can be carried out in a wide range by modifying both the matrix itself and the material embedded in it, for example, technological methods. The creation of composite structures based on matrix and nanocrystals (NC) of a semiconductor is very important. Composite structures can be created by introducing into the matrix of colloidal solutions of NC with subsequent processing at a certain temperature.

We have developed an original method of colloidal synthesis of monodisperse NC CdTe with high stability, narrow bands of photoluminescence (PL) and high quantum yield. A composite system based on porous silicon (PS), which serves as a matrix, and NC CdTe, which are incorporated into the porous matrix, were obtained. The peculiarity of this system is that both components have PL of different intensities. The large difference in PL intensities and different positions of the radiation bands allowed, comparing the PL spectra of the colloidal solution of NC CdTe, PS and NC CdTe – PS at different stages of introduction of CdTe nanoparticles into the porous silicon surface, to identify the interaction and mutual influence of the two constituent materials.

The colloidal solution of NC CdTe was applied to the surface of the PS sequentially by spraying, drip method and the method of precipitation of particles from a fixed volume and subsequent evaporation at a temperature below 100° C. In order to intensify the process of precipitation of CdTe particles in the solution was introduced isopropyl alcohol, which is a solvent with a low coefficient of sedimentation stability in a number of solvents for this system. The dependence of PL intensity on the density of CdTe particles deposited on the PS surface was measured and the PL spectra of the PS – NC CdTe system were recorded at different stages of CdTe nanoparticle deposition on the porous Si surface.

The introduction of NC CdTe into the porous surface creates a strong stable structure. The planned change of properties of PS and colloidal solutions of NC CdTe by variation of technological methods of synthesis and processing methods will allow to control the physical properties of this composite system in a wide range and to use new principles of design and creation of new generation sensor devices.

The refinement of the crystal structure of complex oxide materials: developing and programming of the algorithm

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In general, the software for analyzing data using the X-ray diffraction method does not include the possibility of using stoichiometric principles between chemical elements and the relations between the occupation of crystallographic positions by atoms.

The aim of the research is to refine the crystal structure of materials that allow isomorphous substitution.

To achieve this aim, the following objectives were set:

- to develop an algorithm for refining the distribution of atoms according to the crystallographic positions, taking into account the use of the stoichiometric principles for the material and assess the unambiguity of the obtained distribution;

– to develop a method for minimizing the function of many variables for finding the minimum of the function χ^2 , which makes it possible to refine the distribution of atoms by crystallographic positions with using the stoichiometric principles;

- to develop the program realization of the proposed algorithm and to check its efficiency on model problems in the analysis of experimental diffractograms.

The algorithm and its program realization for defining the distribution of atoms according to the crystallographic positions using stoichiometric principles in materials with isomorphous substitution are developed by the authors. A combination of using the developed algorithm and the FullProf program is proposed for taking into account different conditions that should be satisfied by the distribution of atoms according to the crystallographic positions. The complex method for minimization of a function of the deviation of the theoretically calculated diffractograms from the experimental ones is given to avoid falling of the objective function to a local minimum. Two ways for the difference theoretically minimization of between calculated and experimental diffractograms are proposed. By the first one, with the help of the developed algorithm, the occupation of crystallographic positions can be established, and the minimization method built-in in FullProf calculates all other parameters. By the another way, only the developed algorithm is used and the rest of parameters approximately calculated by FullProf before are fixed. The developed algorithm can be used for any materials in which isomorphous substitution is possible, such as spinels, garnets, perovskites, and others.



POSTER REPORTS Session 3 Physical-chemical properties of thin films



Raman study of photoinduced changes in Cd-doped amorphous GeSe₂ films

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Amorphous GeSe₂ is a well-known semiconductor material extensively studied in view of its photosensitivity and possible applications related mostly to reversible or irreversible photoinduced effects. Doped GeSe₂ glasses and films are much less investigated.

1.2–1.6 [m thick GeSe₂ films doped with Cd (nominal content up to 8 %) were prepared by thermal evaporation on silicate glass and Si substrates. Optical absorption spectra of the films were measured using a Cary 50 spectrometer (Varian). Micro-Raman measurements were performed at room temperature using a Horiba LabRAM spectrometer and solid-state lasers (λ_{exc} =488.0 or 514.7 nm).

Micro-Raman measurements at laser power densities $P_{exc} < 100 \text{ kW/cm}^2$ clearly confirm the amorphous character of the film structure. The observed Raman spectra of the Cd-doped films basically reproduce that of undoped GeSe₂ films with relatively broad features near 175, 200, 215, 265, and 310 cm⁻¹. For the Cd-doped films a new sharp peak near 210 cm⁻¹ appears with increasing $P_{\text{exc.}}$ Its spectral position coincides with LO phonon frequency of crystalline CdSe. The onset power density for the appearance of this peak is lower for higher Cd content while the band positions and intensities depend on P_{exc} and λ_{exc} . This new peak appears within the illumination time of several seconds and does not disappear after the excitation power is lowered again, which suggests that the light-induced local photostructural changes in the film are quite fast and irreversible. The emerging features can be explained by the formation of CdSe nanocrystals in the laser spot area. High- P_{exc} illumination leads to a photoinduced non-thermal drastic drop of the film viscosity in the laser spot, local fluidization of the amorphous GeSe₂ film, and a radial mass transfer from the laser spot. Dynamic breakage and rearrangement of chemical bonds in the photosoftened medium result in an enhanced diffusion of Cd and Se in the illuminated area and facilitates the CdSe nanocrystal formation.

Characterization of Ag–In–S films prepared by thermal evaporation

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Ternary compounds of the Ag–In–S system, in particular $AgInS_2$, are semiconductor materials used for optoelectronic and photovoltaic device applications. Therefore, $AgInS_2$ films prepared by various techniques attract broad scientific interest [1,2]. Here we report on Ag–In–S films with different elemental composition prepared by thermal evaporation.

The structure of the films was characterised by X-ray diffraction using a Rigaku Smartlab X-Ray diffractometer with Cu K_{α} radiation in a Bragg-Brentano geometry. The diffractograms of the Ag–In–S films of different composition revealed reflexes characteristic for AgInS₂ and/or AgIn₅S₈ crystals as well as broad maxima typical for amorphous materials. Thus there is evidence for the presence of crystalline and amorphous phases in the films. The film surface topology studied by atomic force microscopy using an Agilent AFM showed a uniform surface with mean surface roughness from 4.5 to 11.2 nm.

Raman scattering measurements were carried out at room temperature using a Horiba LabRAM 800 spectrometer. Excitation was provided by a Cobolt Fandango solid-state laser with an excitation wavelength of 514.7 nm. The scattered light was detected by a cooled CCD camera. The instrumental resolution was better than 2.5 cm⁻¹. In general, the features in the Raman spectra of the films are noticeably broader than for the corresponding polycrystalline samples which is explained by the presence of an amorphous phase in the films. The dependence of the Raman spectra on the film composition as well as correlations of the observed peak frequencies with those of AgInS₂ and AgIn₅S₈ crystals are discussed.

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Adsorption of thin films of organic peroxides on the amourphous alloys for the drugs immobilization

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Intensive development of nanotechnology is associated with the modification of polymeric and metallic surfaces in order to provide them the specific physico-chemical properties. An alternative activation method is formation of a grafted thin polymeric films from macromolecules of heterofunctional oligoperoxide (HFO). Such oligoperoxides can produce radicals at low temperatures, so they can be used for modification of the amorphous metallic alloy's (AMA) surface [1].

The affinity of HFO macromolecules to solid surfaces leads to the localization of peroxide groups in the interphase. Surface activity of heterofunctional oligoperoxids can be used in medicine, where surface phenomena occur at the tissues interphace. By formation of interphase layers with a predestinate structure and nature it is possible to receive thin polymeric films with the required properties [2].

It was investigated wetting of surfaces of the amorphous metallic alloys (AMA) based on iron and cobalt with aqueous-ammonium solutions of oligoperoxides based on vinyl acetate, 2-tert-butylperoxy-2-methyl-5-hexen-3-yne and maleic anhydride (OP-1) and based on vinyl acetate, 3-tert-butylperoxy-3-phenylbutylmethacrylate and maleic anhydride (OP-2). The surface tension of aqueous-ammonia solutions of oligoperoxides was determined and were calculated values of the macromolecules adsorption. A higher surface activity of OP-2 was observed in comparison with OP-1. The values of the adhesion work between contact and external metallic surfaces and solutions of oligomers were calculated.

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First-principle calculations of band energy structure of CdSeS solid state solution thin films

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The theoretical calculations were performed within the framework of the density functional theory (DFT). The Vanderbilt's ultrasoft pseudopotentials were used for the ion potentials. To describe the exchange-correlation energy of the electronic subsystem, a functional in the approximation of generalized gradient (GGA) and the Purdue–Burke–Ernzerhof (PBEsol) parameterization was used. As a correlation potential, the Ceperlay–Alder and Gell–Mann–Brueckner equations were applied to the high electron-density boundaries.

The charge-density distribution was calculated by the method of special points involving the techniques of charge damping. The relaxation of ion positions on the basis of calculated atomic forces was achieved for each crystal structure, and then the integral stress of the cell was determined. The atomic coordinates and the unit cell parameters were optimized using the Broyden–Fletcher–Goldfarb–Shanno (BFGS) method.

The models of thin films were formed from a three-dimensional crystal along the $[0\ 0\ 1]$ axis. The distance between the formula units was increased by approximately 15 nm, thus forming a vacuum gap to avoid interaction between the layers.

Observation of long-range effect in ion-implanted polymers

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Long-range effect (LRE), which is known for ion-implanted crystals of diamond, metals and semiconductors [1-4], has also been found in ion-implanted polymers, for the first time to our knowledge. The effect is that a change in the physical characteristics of the material is observed far beyond the region of ion penetration into the sample. The present study was performed with polymethylmethacrylate (PMMA) implanted with 40 keV B⁺ ions with different fluences of ions and current density less than 2 μ A/cm². The samples were studied by nanoindentation technique and positron annihilation lifetime spectroscopy (PALS). It was found that the changes of nanohardness induced by ion irradiation are observed up to a distance of about 1300 nm from the surface. This distance is much larger the size of implanted region that is of about 400 nm. The obtained PALS results testify that the microstructural changes occur far beyond the implanted layer of polymer. In addition, the observation of LRE in B⁺-implanted PMMA is also confirmed with FTIR spectroscopy.

The mechanism of the LRE is considered within the Kosevich's model [5], according to which residual mechanical stresses lead to formation of an additional concentration of structural defects far beyond the implanted area.

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Photoinduced changes of optical characteristics of amorphous As–S film-based waveguides

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Amorphous films of As–S system reveal a number of interesting photoinduced effects and are promising materials for modern optoelectronics and photonics as well as for the fabrication of elements of integrated optics [1]. Using a highly sensitive waveguide method with prism-coupling configuration, we studied photostimulated dynamic and irreversible changes of the refractive index n_f as well as photoinduced variation of attenuation parameter for optical guiding modes in As_xS_{1-x} films (0,15≤x≤0,30) under above-bandgap laser illumination (λ =480 nm). Variation of n_f was determined with an accuracy of 10⁻⁴. At the initial stage of the sample exposure to light n_f shortly decreases by a value of the order of 10⁻³ followed by a monotonous increase of n_f until a state of saturation is achieved. If the illumination is interrupted, a similar behaviour of n_f is observed (short decrease followed by a monotonous increase).

The dynamic variation of the film n_f is accompanied by a so-called stopping effect [2] consisting in a sharply increasing attenuation of a waveguide mode under continuous pumping by the above-bandgap light. Dynamics of variation of the waveguide mode attenuation is determined by the competition of two independent processes: external optical recording with a long-term (at least several hours) memory effect and an active function of the assisting waveguide mode by virtue of removal of the preceding optical record (reproduction of the preceding value of attenuation of optical modes in the waveguide stimulated by the light with λ =633 nm).

Comparison of the kinetics of the photoinduced non-monotonous changes of n_f and specific features of the stopping effect revealed a similar dynamics in their behaviour caused by the character of generation and recombination of excited electrons self-trapped on deep levels, their interaction with excitons forming a polaron potentional well. The active role of the assisting light is due to its absorption by these electrons and their transition to the conduction band.

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Effect of chemical treatment of *p*-PbTe plates on electrical properties of structures Cu/*p*-PbTe/Cu

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Lead telluride and solid solutions based on it are widely used for the manufacture of injection lasers in the spectrum of $3-5 \mu m$. Highly doped PbTe is also a promising material for thermoelectricity [1]. The efficiency of devices based on lead telluride largely depends on the quality of electrical contacts.

In our experiments, the Bridgman-grown no crystallographic oriented single crystals of PbTe have been used. PbTe – *p*-type, $[p] = 1.5 \times 10^{18}$ cm⁻³, $\mu_p = 650$ cm²/(V×s), undoped. Technological scheme of PbTe plates processing with etching composition H₂O₂ + HBr + EG is given in [2]. Contacts have been formed on chemically etched surface of *p*-PbTe single crystals by electrolysis deposition of copper. Pre-deposition surface treatment produced interfaces free from oxide layers. All measurements of the I–V characteristics were carried out by the *dc* method in the temperature range 77–295 K on PbTe samples after cutting and chemical-dynamic polishing (CDP).

Figure 1 shows the experimental results of measuring the I-V characteristics of Cu/*p*-PbTe/Cu structures at temperatures of 70 K and 292 K depending on the surface treatment of PbTe.

It should be noted the linearity of the corresponding I-V characteristics throughout the studied temperature range. The chemical deposition of Cu metal on the *p*-PbTe results in ohmic contacts.



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Photosensitivity of CdTe films

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CdTe films deposited at $T_p = 473$ K are photosensitive. Since the absorption coefficient is almost inversely proportional to the thickness, the film thickness is taken to be 400 nm for better absorption of incident light on the films. It was found that the volt-ampere characteristics of CdTe films measured at different ambient temperatures T in the dark and under light are ohmic. The dark conductivity of the grown CdTe films, measured at room temperature, is 10^6 Ohm⁻¹m⁻¹. Dark conductivity as well as photosensitivity increase with increasing T_p in the range of 303–573 K.

Photosensitivity is an effective parameter in determining photoconductivity. Photosensitivity largely depends on natural and external imperfections, which can act as centers of capture or as centers of recombination. Polycrystalline film contains a large number of grains and grain boundaries. At the grain boundary there is a large number of defects and broken atomic bonds, which form additional energy states. These energy states effectively capture charge carriers, thereby creating a potential barrier at the grain boundary.

Photosensitivity largely depends on structural defects, which can act as centers of capture or recombination. In CdTe polycrystalline films, the photoconductivity is determined mainly by processes at the grain boundaries. Based on the results of AFM research, the average size of crystallites was determined and the photosensitivity of films of different thickness and structural perfection was also determined [1].

The photosensitivity of films obtained on polished glass substrates is much higher than for films obtained on fresh chips of mica (111) and increases with decreasing film thickness. This is due to the fact that the specific contribution of grain boundaries increases with decreasing crystallite size [1]. Photoactivation energies decrease in the dark with increasing white light intensity. This decrease in the photoactivation energy at a higher level of illumination is primarily explained by the decrease in the intercrystalline limit potential of the barrier height. It is expected that the potential barrier, in fact, strongly affects the mobility of carriers and thus controls photosensitivity.

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Thermally stimulated and electronically stimulated desorption from the surface of MgO films

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Nanopowder-based materials are increasingly used in science and technology. One of their main characteristics is gas saturation. Therefore, it is important to determine the qualitative and quantitative composition of gas molecules adsorbed on the surface. The most informative method of studying of gas emissions is mass spectrometry.

Using a radio-frequency mass spectrometer ROMS, the analysis of the composition and intensity of thermally stimulated desorption (TSD) from MgO films obtained in vacuum 10^{-5} Pa by aerosol application to a molybdenum substrate. The temperature dependence of the TSD amplitude and the kinetics of components' release in the temperature range of 293-770 K were investigated. The heating rate was 0.2 deg / s.

Electron-stimulated desorption (ESD) studies from MgO films were performed in a special lamp, where an omegatron sensor was used as a mass analyzer. The experiments were performed under a static vacuum. During the research, the pressure of 10^{-9} Pa was maintained in the lamp by means of titanium absorption pumps.

Heat treatment of films in vacuum for 60 minutes at 570 K leads to the remaining of the TSD H₂, H₂O, C₂O at the background level and significant reduce of the release intensity at temperatures above 620 K in the temperature range of 300-620 K. However the release of CO does not change significantly. The release is due to the chemical reactions that undergo at the adsorbed layer. Hydrogen and carbon from the near-surface region releases at temperatures above 620 K, interacts with oxygen and desorbs as CO, H₂O and C₂O. In addition, starting from 670 K the decomposition of Mg(OH)₂ passes with the release of H₂O. MgO films were heated in vacuum before irradiation at a temperature of 570 K for 60 minutes. Electron irradiation (E = 2 keV, j = 1-5 A /m2) was performed at room temperature. An increase in the amplitude of CO ions and the release of gas with mass 16 take place during electron irradiation. The mass 16 corresponds to CH₄, not O, as there is no increase of O₂. A decrease in carbon on the surface during electron irradiation was observed by Auger-analysis. In addition, the diffusion of hydrogen and carbon occurs under electron irradiation. Methane is generated as a result of their interaction. The efficiency of this process stabilizes over time and subsequent electron irradiation does not increase the intensity of emissions.

Flooding processes in the Gd-Fe system

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In modern materials science, a new direction of chemical and thermal treatment of metals is intensively developing, which consists in the use of hydrogen as a technological environment in the process of processing functional materials. Such hydrogen technologies are based on the laws of the influence of hydrogen on phase transformations in metals, including polymorphism, atomic ordering and the formation and decay of intermetallic phases and hydrides. A known process that affects the formation of the phase-structural state of the material is HDDR (hydrogenation, disproportionation, desorption, recombination). If you complete the HDDR process at different stages, you can get very different results.

The Gd-Fe₂ compounds and films and two flood schemes were used for the study -1) The crushed Gd-Fe₂ samples were under a pressure of $2x10^6$ Pa for 168 hours at room temperature. 2) The crushed samples of Gd-Fe₂ were under a pressure of 10⁶ Pa for 30 minutes at temperatures of about 700K. In the first case, hydrogen penetrated the lattice, deforming it. The amount of absorbed hydrogen depends on how finely ground our powder, in the case of thin films, the amount of absorbed hydrogen increases sharply compared to the mass of the "absorber". Electrographic studies of films before and after flooding indicate that such films have become finer. When heating the flooded samples, the reverse process of hydrogen evolution was observed, as evidenced by chemical analysis of the air in the heating chamber. It is possible to use such multi-layered structures to create hydrogen batteries. In the second case, hydrogen reacts with Gd-Fe₂ to form GdH₂ and GdH₃ plus free Fe. As evidenced by the destruction of the sample (turned into powder) and diffraction studies. Unfortunately, the second method is not very productive for films. But such hydrogen treatment can be used to influence the magnetic properties of the obtained powders, because it forms an anisotropic structure of magnetic materials.

Direct surface relief formation on As-S-Zn chalcogenide thin films

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Chalcogenide thin films are very promising materials due to the different applications that use their ability to obtain directly during recording surface relief [1]. The interaction of these films with the electron beam is of interest due to diversity of physical phenomena induced in chalcogenide films.

The purpose of this study is to investigate direct (without selective etching) surface relief formation of optical elements periodic nanostructures on thermal vacuum evaporated film $As_{63.5}S_{35.5}Zn_1$ of ~4,5 µm thickness using electron beam lithography, as well as investigate the changes in surface nanostructures height and shape depending on exposure.

The chemical composition of films was determined by energy dispersive analysis of X-rays. An electron beam using a scanning electron microscope irradiated the films. The influence of electron beam irradiation on $As_{63.5}S_{35.5}Zn_1$ amorphous chalcogenide thin films was investigated. Surface relief of the film was tapped by atomic force microscope.

Formed nanostructures with a height of approximately 2 μ m were detected on As_{63.5}S_{35.5}Zn₁ films after e-beam irradiation. The cones on the surface of films have Gaussian profiles. The exposure dose *G* varied from 12 mC·cm⁻² μ C·cm-2 to 12 C·cm⁻² μ C·cm-2. The dependences of the height of surface nanostructures on the dose of irradiation were analyzed. The changing of shape and parameters of the recorded surface relief on As_{63.5}S_{35.5}Zn₁ films can be explained by the charge model [2]. Charge relaxation time, and initial and inverse doses, and size of interaction region have been determined.

Thus, our investigations have demonstrated that studied $As_{63.5}S_{35.5}Zn_1$ composition is suitable for e-beam recording. These results show that $As_{63.5}S_{35.5}Zn_1$ films can be used for fabrication of the optical elements.

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Structural Disorder and Optical Properties of Electon-Irradiated As₂S₃(Se₃) Chalcogenide Glasses

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Glassy chalcogenides of arsenium are characterized by high transparency in a near and middle infrared and belong to a class of materials which are used as active or passive elements in optical engineering. Experimental studies of the influence of radiation load (gamma radiation, X–radiation or electron radiation) enable to determine the character and change of physical properties of these materials, boundary doses of radiation, to learn the nature and mechanisms of radiational defect–formation, reveal conditions of renewing the initial parameters.

In Fig. the correlation between optical pseudogap E_g^* and exponencial Urbach tail *W* for glassy As₂S₃(Se₃) in dependence of the nature of disorder due to various external factors.



This correlation shows that the optical pseudogap E_g^* and W – this being more important–the slope of an exponential portion of the edge are changing in dependence of the disorder degree. A linear relation between E_g^* and W for chalcogenide glasses As₂S₃(Se₃) is fulfilled practically in the whole range of the values of W energies which was studied up to this time. Thus it can be stated that in this case for these materials the contribution of the structural ("intrinsic" and induced) and the thermal contributions into a change of disorder potential is adequate, and the change of the slope probably reflects the change of the distribution of the states in the tails of zones.

Strong correlation effects if vanadium oxide films

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Vanadium oxides are known to be archetype examples of strongly correlated eletron systems in which effects of antiferromagnetic ordering and Mott-Hubbard transition under the external pressure or doping are realised [1]. Experimental studies of these strongly correlated systems were carried out in a number of works (see [2] for a review). However recently, completely new properties of these well studied compounds were discovered and these findings suggest new applications of these systems [3], in particular, as thin film devices with controlled phase transitions.

In the present work the metal-insulator transition is studied within a doubly orbitally degenerated model of quasi-two-dimensional material based on V_2O_3 film, in which a crucial role is played by on-site Coulomb interaction and correlated hopping of electrons, the latter responsible for the electron-hole asymmetry. A model, which takes into account the orbital degeneracy but neglects the correlated hopping has been used for theoretical description of perovskite oxides very recently [4]. With use of a projection procedure in the Green function method the energy spectrum of electrons has been calculated to model variaions of material properties at the temperature changes, the external pressure application or doping. The obtained expressions for thermodynamic potential and the energy gap width allow us analysing the possible phase transitions in a system and the dependencies of characteristics on the external actions as well as classifying factors which determine the electron conductivity and the magnetic properties of these strongly correlated materials.

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Influence of Auxeticity on the Formation of Stress Fields Near Linear Defects in Silicon

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It is well known that silicon crystals, widely used in optical instrumentation, functional acoustoelectronics and radio engineering, have auxetic properties in almost the entire temperature range of its existence: from partially auxetic in the range of 0-600 K to fully auxetic at temperatures of about 844 K. Deformation mechanisms such crystals have not been studied to date. This is especially true of the partially auxetic modification, in which "auxetic" and "non-auxetic" dislocations coexist in different crystallographic directions, which behave differently in the external mechanical field [1], creating significant energy obstacles for each other.

The paper presents the results of studies of the distribution of mechanical stress fields near linear defects in the auxetic and non-auxetic directions in silica in a wide temperature range. It is shown that in the directions with positive and negative values of Poisson's ratios (v) in the crystal the magnitudes of the stress fields around the edge dislocations differ several times (sometimes by an order of magnitude) and are rotated in space relative to the dislocation nucleus by almost 90°, which leads to difficulty movement of dislocation segments in the process of their plastic deformation (See Fig).



Spatial distribution of the component of the tensor of mechanical stresses σ_{zz} around the edge dislocation in α -SiO₂ in the ordinary (left - $\nu = 0.15$); and auxetic (right - $\nu = -0.55$) directions in the crystal.

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Direct Surface Formation in Amorphous As₂₀Se₈₀ Films by Polarization Holography

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Amorphous chalcogenide-containing photosensitive thin films (CPF) show photo-induced mass transport (PMT), i.e. lateral movement of the material under band-gap light irradiation. During single beam or holographic exposure with light interference patterns (IP) these films deforms following the distribution of intensity or polarization of the IP resulting in the formation of so-called surface relief gratings (SRGs). Note that despite to the light-induced softening of glassy matrix the temperature of the film is ambient and the film remains to be in a sold-like state.

The process of SRG formation depends on many parameters such as irradiation intensity and polarization state of recording laser, film compositions and initial film thickness, temperature of recording, polarization of additional irradiation etc.

We report on a systematic study of SRG formation in As₂₀Se₈₀ amorphous films by vectorial (polarization) holography and the results were compared to the kinetic of diffraction efficiency related to the SRG obtained by scalar holography. Four different polarization configurations were used: s-s, p-p (intensity IP) and 45-135, p-s (polarization IP). In addition, we investigated the effect of P or S polarized incoherent assisting light beam.

For the first time to our knowledge, it was detected that with the increase of temperature of recording (from ambient to glass-transition temperature, Tg or even more). PMT in CPF occurs due to variation in polarization across the interference pattern with the rates, which significantly exceed those at room temperature. We have found that the direction of the PMT depends on the direction of light polarization both recording and additional beams not only at ambient temperature but also even near the glass-transition temperature. There results have shown also that the efficiency of surface relief formation is many times higher in the case of 45/135 polarization state of the recording beams in compare to the case of p-p recording. The mechanism of the direct recording of surface relief on amorphous chalcogenide films based on optically induced gradient force model that includes both the spatial distribution of polarization and the anisotropy of the material permittivity is discussed.

Structural changes of As₄₀S_{60-x}Se_x thin films induced by different wavelengths light studied by Raman spectroscopy

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Amorphous chalcogenide glassy (ChG) semiconductors are widely investigated and applied in optics and photonics due to the number of unique characteristic and peculiar effects: wide range of optical transparency, especially in the infrared region, high optical nonlinearity, photoinduced change of optical parameters, and have shown good results in many applications: high density information recording, holography, diffractive optics. The change in optical, structural and surface properties of amorphous chalcogenide thin film upon photoexposure is a well-known phenomenon. The sensitivity and values of these changes mainly depend on chemical compositions of ChG and energy of exposure beam, and both of them can be changed with the aim of optimization or adjustment to the existing task.

Accordingly, better understanding of the structural changes can help in the optimization of the sensitivity on binary As-S(Se)or ternary (As-S-Se) thin films. In most of the previous studies, the exposition by cw Ar⁺, He–Ne or He-Cd lasers (λ =514.5, 632.8 and 440 nm respectively) were used to investigate changes in optical/structural/surface properties. In details the origin of photoinduced effects is not still fully understood especially for different light sources.

The aim of this work is to investigate changes in structural properties induced on ternary amorphous $As_{40}S_{60-x}Se_x$ (x=0, 20, 30, 40, 60) thin films by annealing and exposure by different wavelength light (beams of light emitter diodes with wavelength of λ =375, 405, 450, 525, 570, 630, 690, 740 nm and intensity P=0.1 W/cm²) which either corresponds to the band gap or are above/below this energy value.

The compositional dependence of structural changes under the annealing at 160 C during 12 hours and exposures of a band gap beam of LED diode, as well as above/below this energy value, were studied using Raman spectroscopy. According to Raman spectroscopy the structure of As-S-Se glass consists mainly of AsSe₃, AsS₃ pyramids As₄Se₃ As₄S₄ cages, and S (Se) chains and rings. To resolve overlapping lines responsible for each structural unit the obtained Raman spectra of each sample were decomposed by Voigt profile. The maximum of decomposed profiles shifts toward higher frequency with decreasing Se content showing "two-mode" behavior, similar to observed for CdS_xSe_{1-x} alloy. Thin films' structure move by exposure or by annealing toward the bulk material structure support the idea that both thermally and photo-induced structural relaxation is linked to the polymerization of molecular fragments embedded in the structure of the as-evaporated films.

Synthesis and structural properties of Cu₂ZnSn(S_xSe_{1-x})₄, SnS nanocrystals for printed solar cells

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 $Cu_2ZnSn(S_xSe_{1-x})_4$ (CZTSSe) and SnS compounds are now considered to be one of the most promising materials for the creation of absorbing layers of third-generation thin-film solar cells (SE).

Unlike other semiconductors (GaAs, InP, CdTe, CIGS), which are now used as absorbers of modern thin-film SE, these materials do not contain rare and environmentally hazardous components, and the elements that are part of them are widespread in the earth's crust and are inexpensive to mine.

Previously, we developed a low-energy method for obtaining SE layers with a controlled crystal structure and a minimum content of secondary phases. He includes obtaining them in three stages: colloidal chemical synthesis of nanocrystals (NCs) semiconductors, followed by deposition of nanoinks based on such suspensions on substrates using non-vacuum methods (e.g., 2- or 3-D printing, a spray method, etc.) and, finally, post-growth thermal annealing of samples to remove organic impurities and recrystallize the material.

The work aims to optimize the conditions of NCs synthesis of CZTSSe and SnS compounds by determining their structural-phase state depending on the physicochemical conditions of synthesis.

CZTSSe NCs were obtained by polyol synthesis in triethylene glycol reaction medium. SnS nanocrystals were synthesized using two methods: the polyol synthesis method and precipitation in an aqueous-ammonium solution. The product formed due to the synthesis was selected and separated from the organic component by centrifugation, followed by three washes with isopropyl alcohol. The precipitate was dried in the air in an oven.

To determine the structural properties of the synthesized NCs, an X-ray diffractometer DRON 4-07 was used. Studies of the morphology and elemental composition of the samples were performed using a scanning electron microscope SEM Inspect S50-B, equipped with an energy dispersion spectrometer AZtecOne with a detector X-MaxN20. Raman studies were performed using a RENISHAW in Via Reflex microspectrometer.

As a result of researches, the process of synthesis of single-phase CZTSSe, SnS NCs of the controlled structure is optimized.



POSTER REPORTS Session 4 Thin film compounds for electronic devices, nanoelectronics



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GaP-based UV photodetectors with surface nanostructure

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Surface barrier diodes based on wide-gap semiconductors are promising for use as active elements of shortwave electronics. Among the materials used should be distinguished gallium phosphide, on the basis of which Au-GaP contacts have already been established, the range of photosensitivity of which covers the range of 0.2-0.5 μ m. The main disadvantage of these photodiodes is the relatively low height of the potential barrier ($\phi_0 \leq 1.0$ eV at 300 K), which limits the possibility of their operation at elevated temperatures. This question



Fig.1. The photosensitivity spectra of Ni/GaP/In photodiodes: 1 - with SNS, 2 - with a mirror surface (293 K).

especially becomes important when these structures are used in the photodiode mode, when speed of photodetectors is significantly improved. One of the promising ways that significantly improves the parameters of photodiodes is creation of surface the a nanostructure (SNS) on a semiconductor substrate. We have created Ni/GaP/In photodiodes on gallium phosphide substrates using SNS. The main photoelectric properties are investigated. Base substrates

 $(5 \times 5 \times 0.5 \text{ mm}^3)$ were cut from commercially available n-GaP plates without epitaxial layer, the surface of which after mechanical and chemical polishing was mirror. After additional etching of the substrates in a mixture of KOH + NaNO₃ at a temperature of 400-450 °C during 20 minutes, the surface became matte, and also changed some physical properties. Photodiodes with SNS have a significantly better sensitivity in the UV region of the spectrum than photodiodes with a mirror surface. The maximum sensitivity $S_{\lambda}\approx 0.15$ A/W for Ni/GaP/In structure with SNS was achieved at $\lambda_{max}\approx 320$ nm. The height of the potential barrier Ni/GaP was equal to $\phi_0 \approx 1.45$ eV.

Influence of asymmetric donors on molecular structure-property relationships of the compound containing 4,6-bis(4-chlorophenyl)-2-phenylpyrimidine as acceptor

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Although abundant purely organic thermally activated delayed fluorescence (TADF) emitters have been reported, it is still great challenge to construct highly efficient emitters.^[1,2]

Diphenylamine, tertbytulcarbazole, carbazole,9,9-dimethyl-9,10dihydroacridine, tertbytulacridine and phenothiazine are using as electrondonating moieties for this aim.

In our work phenothiazine and 9,9-dimethyl-9,10-dihydroacridine were used as electron donors.

Phenothiazine has recently been introduced to design TADF materials.^[3] Adachi *et al.* first reported a TADF molecule, PTZ-TRZ, in which the phenothiazine group worked as the electron donor.^[4]

Acridine moieties based on the triarylboron-contained emitters achieved maximum external quantum efficiencies of 12.8% and 17.3%, respectively.^[5]

designed compounds containing 4,6-bis(4-chlorophenyl)-2-The 9,9-dimethyl-9,10phenylpyrimidine acceptor fragments of and as dihydroacridine(HS-5) and phenothiazine(HS-3) as electron-donating moieties were synthesized by Buchwald-Hartwig cross-coupling and by nucleophilic substitution. The structures of the synthesized compounds were confirmed by NMR, IR and mass spectroscopies.

Influence of different donors on molecular structure-property relationships of the compounds was studied by synthesis of compound with asymmetric donors(HS-8).



Fig. 1. Scheme of synthesis of asymmetric derivative HS-8

HS-3 and HS-5 achieved a maximum quantum yield of 5.62% and 37.85%, respectively. PL spectra of HS-8 shows a hypsochromic shift and decreasing of difference in intensity are caused by acridine donor. The difference between not deoxygenated and deoxygenated toluene solutions of compounds confirms TADF.



Fig. 2. PL spectras of not deoxygenated and deoxygenated toluene solution of HS-3(a), HS-5(b) and HS-8(c)



Table 1. Quantum yield and decay time of the synthesized compounds.

Quantum yields, %			
	toluene solution	Decay Time, ns	
HS-3	5.62	2.79	74.13%
		4.20	25.87%
HS-5	37.85	25.97	70%
		555.53	30%
HS-8	32.56	3.19	46.68%
		15.14	53.32%

In general, this systematic study of the relationship between chemical structure and photophysical properties provided a strategy to design highly efficient TADF molecules.

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POSTER REPORTS

Session 5 Functional crystalline materials: growth, physical properties and applications



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Electrophysical Properties of Cadmium Antimonide when Irradiated with ⁶⁰Co Gamma-quanta

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The introduction of radiation defects into the crystal lattice of cadmium antimonide changes its electrophysical properties and makes it possible to control them. Since the technology of growing this type of semiconductors is still imperfect, at low doses of radiation, radiation-induced defects will form various complexes with uncontrolled impurities. This makes it much more difficult to obtain information about the role of intrinsic lattice defects in determining the physical properties of CdSb semiconductors. Radiation centers introduced into the crystal during its irradiation, both at room and nitrogen temperatures, partially "neutralize" the charge of impurity ions localized in the lattice nodes. Moreover, for liquid nitrogen temperatures, this process is more intense than for room.

The effect of radiation defects in specially non-doped and tellurium-, indium-doped crystals of cadmium antimonide before and after high doses of 60 Co ${}^{\gamma}$ -quanta irradiation was studied on the basis of measurements and analysis of temperature dependences of electrical conductivity, Hall effect in the temperature range (78÷295) K. Gamma-irradiation with high doses leads to significant changes in electrophysical properties. The mechanisms responsible for these changes are established and a theoretical explanation of these effects is given.

Irradiation of p-type conductivity samples leads to a decrease in the hole concentration. In the process of further irradiation, the region of full compensation passes, changing the type of conductivity. An increase in the electron concentration in CdSb(Te) and a decrease in CdSb(In) are observed in n-type samples.

The removal of electrons from the conduction band is due to the formation of radiation defects with a deep level in the bandgap of the crystal. Donors with $E_c - 0.16$ eV energy levels, introduced regardless of the type of irradiation and the type of doping impurities, are responsible for their own lattice defects.

The nature of the change in the temperature dependence of the mobility indicates that before irradiation the scattering of current carriers occurs mainly on the lattice, whereas after irradiation the scattering on ionized impurities plays an important role.

Optical studies of high-resistance CdTe crystals and Cd_{1-x}Zn_xTe solid solutions

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To improve the technological processes for the preparation of chalcogenide semiconductor materials and solid solutions based on them, it is necessary to carry out a number of electrical and optical studies in order to assess the effect of deviations from stoichiometry and dopants on the parameters of the material. As a result of research, it is possible to evaluate and subsequently control these parameters in the course of the technological process.

Based on the above results on the study of reflection and transmission spectra in the range of 800-1100 nm, reflection and transmission spectra in the range $(1.4 - 25) \cdot 10^{-6}$ m and photoluminescence spectra at a temperature of 5 K in the energy range 1.35 - 1 7 eV of high-resistance single crystals of CdTe orientation (111) with resistivity $\rho = (2 \div 5) 10^9$ Ohm \cdot cm doped with chlorine, and solid solutions Cd_{1-x} Zn_xTe (x = 0.1) with resistivity $\rho = 5 \cdot 10^9$ Ohm \cdot cm $^{-3} \cdot 10^{10}$ Ohm \cdot cm the following results were obtained:

The energy relaxation time τ (τ =1.01·10⁻¹⁴s) and the effective "optical" mobility μ_{opt} (μ_{opt} =206.45·10⁻⁴ m²V⁻¹s⁻¹) of free charge carriers for high-resistance CdTe (111) single crystals are estimated. It was determined that the energy of the fundamental optical transition E₀ of the materials under study at T= 300 K is as follows, for CdTe 1.44 eV, and for Cd_{1-x}Zn_xTe 1.5 eV. The temperature coefficient of the change in the band gap is estimated, which is $-5.32 \cdot 10^{-4}$ eV/K for CdTe and $-5.2 \cdot 10^{-4}$ eV/K for Cd_{1-x}Zn_xTe (x = 0.1). The relationship between the energy of the fundamental optical transition E0 and the temperature T is established: E₀ (CdTe) = 1.5997 eV - 5.32 \cdot 10⁻⁴ eV/K·T for high-resistance CdTe (111) single crystals and: E₀ (Cd_{1-x}Zn_xTe, x = 0.1) = 1.6562 eV - 5.2 \cdot 10⁻⁴ eV/K·T for solid solutions Cd_{1-x}Zn_xTe (x = 0.1).

It is shown that the crystals under study have a high (detection) quality, which is decisive for the manufacture of highly sensitive and high-precision sensors of ionizing radiation. The practical value of the results obtained lies in the determination of the electronic and physical parameters of the technically important semiconductors CdTe and Cd_{1-x}Zn_xTe.

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Calculation of the vibrational spectra of CdSe and CdS crystals with zinc blende structure

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Semiconductor compounds $A^{II}B^{VI}$ have many important applications in solar cell, efficient thin film transistors and light-emitting diodes [1, 2]. In spite of extensive experimental and theoretical studies of these materials, some of their fundamental parameters are still unknown. On the other hand, this information is very important for modeling and developing different optical and electronic devices. Among numerous theoretical studies of the electronic and phonon band structure [1–4], the optical parameters [3, 4] of CdSe and CdS compounds, we have not found the full results for the temperature behavior of Raman spectra.

The fundamental electron and phonon properties of the CdSe and CdS crystals with cubic structure are studies. Having performed the electronic band-structure calculations for CdSe and CdS, one can obtain their optical parameters. Finally, we have derived the temperature dependence of Raman spectra, free energy, heat capacity, entropy, enthalpy and Debay temperature.

The theoretical calculations were performed within the framework of the density functional theory (DFT). To describe the exchange-correlation energy of the electronic subsystem, a functional in the approximation of generalized gradient (GGA) and the Purdue–Burke–Ernzerhof (PBEsol) parameterization was used.

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Limited thermoelectric figure of merit of n and p-PbTe

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An important task of thermoelectric materials science is the theoretical calculation of extreme values of the dimensionless thermoelectric figure of merit (ZT) of the studied materials. Priority knowledge of such parameters makes it possible to determine whether to work with this material to obtain a given ZT, or whether it is more appropriate to use another matrix. In addition to estimating the maximum possible value of ZT, it is equally important to determine the most effective ways to achieve these values. Such calculations are the theoretical basis for establishing general criteria for finding new materials with high ZT.

The dimensionless thermoelectric figure of merit of n and p-PbTe depending on the chemical potential of electrons μ for different possible dominant scattering mechanisms is calculated taking into account the peculiarities of edges of the energy bands, and degenerate statistics of charge carriers. As a result, the optimal values of μ at which the value of ZT reaches a maximum are established. The influence of various factors on the obtained result is demonstrated. Conclusions have been made about the most effective ways to increase the thermoelectric figure of merit. The conclusions from the calculations can be applied to PbTe, and can be approximated to other semiconductor materials used to convert thermal energy into electrical energy. The most important conclusion is that the potential of PbTe as a thermoelectric material has not been fully realized yet.

Study of absorption spectra of crystals Pb_{1-x}Ge_xTe in the vicinity of the phase transition

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The presence of a phase transition (PT) in narrow-gap compounds of the $A^{IV}B^{VI}$ group is of great interest to researchers, since in the vicinity of the structural PT, when the crystal lattice becomes loose and labile, the properties of crystals are nonlinear and extreme, therefore, various new effects are hidden here.

The study of the intrinsic optical absorption spectra for different temperatures, and, especially, in the vicinity of the phase transition, allows, firstly: to clarify the nature of interband transitions, to clarify the band structure of crystals in both phases, and to determine its possible change during phase transition. Secondly: by studying the intrinsic absorption edge, one can reveal a possible anomaly in the band gap (and, consequently, the form of the phase transition), and from its long-wavelength region, changes in the phonon spectrum of the crystal during phase transition

 $Pb_{1-x}Ge_xTe$ solid solutions, as a rule, have a high concentration of charge carriers, and hence a high absorption coefficient. Therefore, the absorption spectra in the vicinity of the PT have been relatively little studied. We carried out such studies on samples with a low Ge content ($0.03 \le x \le 0.10$), in which the carrier concentration was no more than $(1 \div 3) \cdot 10^{18}$ cm⁻³. The study of the main absorption edge for T < Tc in the range 0.14 eV < hv < Eg additional absorption, which may indicate a possible rearrangement of the electronic spectrum of the crystal in the ferroelectric phase [1], as well as the influence of other factors, which is the cause of blurred, not point-like PT.

To differentiate the additional long-wavelength absorption with the edge of the main absorption in the ferroelectric phase, we studied the temperature dependence of the transmission spectra for a fixed wavelength ($\lambda = 4.77 \mu m$; x = 0.045) in a narrow temperature range that contains the phase transition. The rate of change in transmission with temperature calculated on the basis of the transmission spectra showed a resonant, anomalous character, which, in our opinion, indicates a change in the mechanism of absorption of photons by the crystal in a narrow vicinity of temperature (about 1.5 K) before and after T_c. For a more accurate conclusion, it is desirable to investigate the temperature dependences of the intrinsic absorption edge in both phases.

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Scattering mechanisms in crystals PbS p-type conductivity

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The theoretical analysis of scattering mechanisms of carriers by thermal vibrations of crystal lattice is done. The calculation provided of the mobility of carriers in a wide temperature (4, 2 - 300 K) and concentration $(10^{16} - 10^{20} \text{ sm}^{-3})$ bands in view of interacting conduction of holes of deformation potential acoustic and optical phonons and polarization potential of optical phonons.

Kinetic parameters of semiconductor materials are largely determined by the scattering mechanisms of carriers. Scattering mechanisms of carriers in lead chalcogenides have been studied repeatedly by different authors. But despite this, at present there is no consensus on the concentration and temperature limits the dominance of certain types of scattering. In this paper, based on comparison of theoretical calculations with the experimental Hall mobility data of specified concentration and temperature limits the use of approximate models of the band structure and the prevailing scattering mechanisms of charge carriers in lead selenide crystals p-type conductivity.

The dominant scattering mechanisms of carriers in hole lead selenide crystals are the scattering of short-range potential vacancies for the concentrations of $10^{19} - 10^{20}$ sm⁻³ and the lattice thermal vibrations.

Scattering of phonons gives a correct picture of the quality necessary to characterize transport phenomena. The role of polar optical phonon significant at temperatures of 77 and 300 K for concentrations of $10^{16} - 10^{18}$ sm⁻³. When increasing the concentration scattering on optical phonons is reduced due to screening.

At high concentrations (higher 10¹⁹ sm⁻³) scattering on optical phonons is manifested through their deformation potential, whose influence on the total scattering at certain concentrations is very essential at room temperature. Scattering of carriers by acoustic phonons significant for all temperatures in the considering the whole studied concentration range. For temperature 77 K influence on the total scattering dominates deformation potential scattering on optical phonons.

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Levels of acceptor's impurities in β-Ga₂O₃ nanostructures

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 β -Ga₂O₃ has attracted significant interest as a semiconductor for power electronic and radio frequency applications. Unintentionally doped β -Ga₂O₃3 is typically n-type which is attributed to Si, Sn and Ge, and also, but less studied, with Ta and Nb impurities [1]. A major drawback of β -Ga₂O₃ till present has been lack of a reliable method for fabricating p-type β -Ga₂O₃. This is a key limitation for it's entry into a whole range of semiconductor device markets. Indeed, it is generally proposed that useful levels of majority acceptor (p-type) doping in β -Ga₂O₃ are unlikely to be obtained because of a combination of factors including the relatively low absolute energy level of the valence band, the lack of an identified shallow acceptor, the relatively high effective masses of holes at the top of the valence band, the propensity for self-trapping of holes and the relatively low formation energy of the oxygen vacancy donor which favors compensation of acceptors. Although, to the best of our knowledge, there are no direct demonstrations of impurity-doped p-type β -Ga₂O₃ in the literature several studies have, nevertheless, evoked the possibility of p-type doping [1].

The objective of this work is to investigate, using density-functional-theory calculations, the efficiency of doping with Mg, Ca, Bi, Zn to raise the valence band of β -Ga₂O₃ nanostructures to a level at which p-type doping is achievable.



Fig. 1 – Occupied states of valence electrons at 0 Kelvin in the β - Ga₂O₃ 30 atoms pure cluster and with Mg impurity at a concentration of 7.1%. The abscissa is atomic units of energy; the ordinate is a number of states

The graphs in Fig. 1 show an increase in the density of states of the valence band of a cluster with an Mg impurity in the region of the band top. In this case, the distance to the first unoccupied state of a pure cluster was 212.9 eV, and with an Mg impurity it was only 1.6 eV.

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Vapor phase growth and properties of mixed layered Pb_{1-x}Cd_xI₂ semiconductors

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Heterogeneous solid solutions of $Pb_{1-x}Cd_xI_2$ are characterized by intensive photo- and X-luminescence at room temperature and high radiation resistance, while it opens up a possibility of using these materials for the production of high efficient rapid-action non-cooled scintillation detectors of ionizing radiation [1].

Peculiarities of growing mixed layered $Pb_{1-x}Cd_xI_2$ crystals (x=0,1; 0,9) from vapor phase in an enclosed system at over-stoichiometric iodine vapor pressure has been researched. Lead and cadmium iodides were synthesized from separate components. Iodides alloy was used as a vaporization source. For growth of $Pb_{0.1}Cd_{0.9}I_2$ semiconductors temperature gradient has to be higher than gradient for $Pb_{0.9}Cd_{0.1}I_2$.

An X-ray diffraction analysis of the grown crystals has been done and it was found that 4H-modification crystals with crystal lattice parameters: for $Pb_{0.9}Cd_{0.1}I_2$ a= 4,529(7) A, c= 13,96(4) A, V= 247,9 A³; for $Pb_{0.1}Cd_{0.9}I_2$ a= 4,258(3) A, c= 13,702 A, V= 215,04 A³. The decrease in the volume of the unit cell with increasing Cd content in crystals can be explained by the substitution of Pb atoms by Cd atoms, ie the formation of solid substitution solutions.

The morphology and quality of the crystals grown were studied using both optical microscope and scanning electron microscope. The light yellow $Pb_{0.9}Cd_{0.1}I_2$ crystals grew in the form of plates and ribbons, the surface of which is sculpted by growth figures, and the transparent $Pb_{0.1}Cd_{0.9}I_2$ crystals grew from the vapor phase only in the form of plates. Kinematic waves of stairs density are observed on the surface of some crystals, which are a collective effect due to the influence on the movement of the echelon of stairs of various disturbances.

The spectral dependences of optical absorption of grown $Pb_{1-x}Cd_xI_2$ crystals (x=0,1; 0,9) at room temperature are researched. By the crystals' absorption spectra the values of the crystals band gap have been obtained by means of Tauc relation.

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Structures with piezophotron effect

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The field of studying the piezophototron effect in semiconductor thin films is new. Using materials that are simultaneously semiconductors, piezoelectrics and have photoelectric properties makes it possible to create a fundamentally new class of semiconductor devices, especially in the field of sensorics and photovoltaics. The production of films of the A_2B_6 group, which include CdS, CdTe, CdSe, ZnS, ZnSe, ZnO with an available piezoelectric effect, is an urgent task. In this work, the object of study is diode structures based on semiconductor films. We studied structures exactly with CdS, CdTe, CdSe, ZnS, ZnSe films grown by thermal evaporation on a flexible molybdenum substrate. An example of the structure under study is shown in Fig. 1. The study of the piezophototron effect of the structures was carried out by measuring the current-voltage characteristics (I-V) under illumination and in the dark, without pressure / when pressure is applied to the structure, as well as when twisting. An example of the obtained I - V characteristics is shown in Fig. 2.



Fig. 2. Dark I - V characteristics of the Mo-CdS-Cu_xS structure.

From the obtained I - V characteristics, it was determined that a rectifying barrier is formed between the semiconductor films and the structure has a diode characteristic. An increase in the reverse and forward currents was found with increasing pressure, which allows us to conclude that there is a piezophototron effect.

Single crystals growth of silver-containing thio-compounds with argyrodite structure

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Compounds with argyrodite structure are the promising materials for the effective solid-state batteries. The aim of this work is to develop the fundamental bases for obtaining new solid electrolytes based on modified silvercontaining thio-compounds with the argyrodite structure and to optimize the technologies for single crystals growth.

Single crystals of solid solutions of Ag₇SiS₅I-Ag₇GeS₅I system were grown from pre-synthesized polycrystalline alloys. Synthesis of selected compositions was performed in evacuated to 0.13 Pa quartz ampoules from previously obtained silver-containing thio-compounds taken in stoichiometric ratios. The heating was performed in two steps: first to 723 K (exposure for 48 h) and then to maximal temperature 1273 K (72 h). Cooling to the experimentally selected annealing temperature of 873 K was carried out at a rate of 100 K/h with the following homogenizing annealing for 120 h. Cooling to room temperature was carried out in furnace-off mode. Such obtained alloys of solid solutions were investigated by differential thermal analysis (Pt-PtRh X-ray thermocouple) powder diffraction method (DRON-4.07 and diffractometer, Ni filtered CuKa radiation).

Single crystals of $Ag_7Si_xGe_{1-x}S_5I$ solid solutions were grown by crystallization from a melt-solution technique. Growth was performed using conical quartz containers in a vertical two-zone tubular resistance furnace. Since the melting temperatures of $Ag_7Si_xGe_{1-x}S_5I$ solid solutions are similar and within 1166 and 1172 K, the temperature regime of grown crystals is the same. Formation of the crystalline seed was carried out by the solid-state recrystallization method for 48 h. The optimal velocity of the crystallization front was 0.4-0.5 mm/h, the cooling rate to room temperature - 5 K/h.

As a result, the technological regimes of obtaining high-quality single crystals of solid solutions based on quaternary silver-containing thio-compounds Ag_7SiS_5I and Ag_7GeS_5I were optimized. By this method were obtained single crystals of $Ag_7Si_xGe_{1-x}S_5I$ solid solutions with composition x = 0.2, 0.4, 0.6, 0.8. Grown samples were 30–40 mm long and 10–12 mm in diameter with a dark gray color and a metallic luster.



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Electrocatalytic Mo-rich superalloys: synthesis and morphology characterization

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The design of effective cathode materials for hydrogen evolution reaction (HER) has been focused on Mo alloys with iron group metals (Ni, Co, Fe) due to their superior catalytic performance in alkaline media, reasonable corrosion and oxidation resistance, stability at elevated temperatures. The catalytic activity for hydrogen evolution is qualitatively proportional to the Mo content in Mobased alloys. Our efforts were directed to optimize the plating bath vs. deposition conditions in order to obtain electrolytic Mo-rich alloys as effective catalysts for the HER.

The selection of ammonia-acetate electrolyte was inspired by the assumption that the deposits with a high Mo content can be deposited [1-3].



Fig.1. SEM of Ni-Mo alloys, deposited at current densities, mA cm⁻²: 30 (a) and 300 (b).

Smooth and crack-free Ni–54 at.%

Mo alloys have been prepared at 30 mA cm⁻² (Fig.1).

It was found that the Mo content in Ni–Mo alloys can be tuned to 78 at.% by decreasing the molar ratio $[Ni^{2+}]/[MoO_4^{2-}]$ in the electrolyte to 0.25 and increasing the cathodic current density to 300 mA cm⁻². However, dense cracks and pits are formed due to hydrogen evolution at high current densities and that diminishes the catalytic activity of the coating for HER.

Acknowledgment. This work was carried out in the framework of the target research program of the NAS of Ukraine "New Functional Substances and Materials of Chemical Engineering", project №7–21, 2021.

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Influence of hard ultraviolet on solar cells characteristics based on CdTe obtained by thermal evaporation

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The investigations are devoted to the research of hard ultraviolet (UV) irradiation on structure and optical properties of thermal evaporated CdTe films and output parameters, light diode characteristics of film solar cells made on them. To study the effect of hard UV irradiation on the structural properties of CdTe films and solar cells, they were irradiated with hard UV irradiation with quantum energy of 10 eV, a luminous flux density of 10^{20} - 10^{21} quanta/m²s for 8 hours.

It is established that the action of hard UV irradiation on thin films of cadmium telluride obtained by thermal evaporation does not affect the optical properties of thin films, but changes their structural properties. In these films the level of macrostresses has increased and the level of microstresses has decreased by $\approx 10\%$.

It was found, that according to the results of analytical processing of the light JV characteristics of the solar cells after hard UV irradiation, it is seen that the values of the photocurrent density and the short-circuit current density has slightly decreased for solar cells obtained by thermal evaporation. There is a stability of the open-circuit voltage value in solar cells after hard UV irradiation. For the solar cells sample the efficiency parameter value has decreased by 0.08 arb. units. The negative impact on efficiency of solar cells was a decreasing in the values of the photocurrent density and the short-circuit current density by 12% and 11%, respectively, as well as an increasing diode saturation current value in 2 times.

This behavior of the output parameters and light diode characteristics of solar cells obtained by thermal evaporation can be explained by the presence of a certain number of crystalline defects in the CdTe absorbing layer. The accumulation of electroneutral point defects on the developed grain boundary surface after obtaining the CdTe layer and electroactive point defects after diffusion chloride treatment limits the rate of Cu atoms the to CdS/CdS_{1-x}Te_x/CdTe heterostructure. This is a well-known problem of CdTe solar cells output parameters degradation. Obtaining a base layer of CdTe by vacuum methods allows obtaining standard values of crystal grain size at the level of 1-10 µm, but this can be a significant cause of degradation of solar cells based on such layers due to diffusion of copper atoms on the columnar structure of CdTe layer. The prolongation of the stable work time of such devices in space with ionizing radiation, such as hard UV light, is associated with a decrease in grain size in the CdTe layers.

Obtaining and thermoelectric properties semiconductor materials-based systems Pb-Sb-Te, Pb-Bi-Te

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The priority of world scientific research is the development of energy-saving technologies, the creation of efficient renewable energy sources. At the same time, research related to the conversion of thermal energy into electricity comes to the fore.

The efficiency of thermoelectric materials is determined by the thermoelectric figure of merit (ZT), which is related to the Seebeck coefficient, specific conductivity, thermal conductivity and absolute temperature. Note that the most common modern thermoelectric generators operate on the basis of materials for which ZT ~ (0.6 - 1.0). Therefore, increasing this parameter to the values of ZT ~ (1.5 - 2.0) will significantly expand the scope of thermoelectric converters.

The main ways to obtain materials with a high value of ZT is to search for new materials or modify the properties of already known. Among the materials now used for the manufacture of heat generators, it should be noted lead telluride (PbTe), for which in the undoped state ZT ~ (0.7 - 0.8). However, its basic parameters can be effectively changed by doping and creating solid solutions. A particularly promising impurity is antimony, which, replacing lead ions, gives an electron to its conduction band, which causes an increase in the concentration of free electrons and specific conductivity. In solid solutions of PbTe-Sb₂Te₃, the thermoelectric properties can be further improved by reducing the thermal conductivity due to the scattering of phonons on the point defects of the crystal lattice.

The technological bases of synthesis and formation of thermoelectric samples based on PbTe doped with Sb and Vi by the method of pressing powdered material with fractions of micro- and nano-sizes, which cause the formation of a significant number of internal boundaries for additional phonon scattering, are carried out. However, to improve the thermoelectric properties of the material, it is necessary not only to reduce the thermal conductivity, but also to increase the Seebeck coefficient. This can be achieved if conductive nanochannels are formed around PbTe grains with a size of $(0.4 - 1.0 \ \mu\text{m})$ by introducing colloidal silver particles. It is established that the introduction of Ag nanoparticles with sizes (40 - 60) nm not only reduces the thermal conductivity to (0.08 - 0.2) W/m K, but also leads to an increase in the Seebeck coefficient to 320 μ V / K due to additional electron throttling barriers formed by silver nanoparticles.

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Features of the fabrication and properties of thin-film energy converters based on doped PbTe

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Recently, more and more micro-sized devices have appeared in the electronics industry, for the operation of which several microwatts of power are enough. Thin-film thermoelectric generators TTEG can be used as an onboard power supply due to its small size. Additionally, there is possibility to apply TTEG in biomedical equipment, implanted devices, power supply systems, for temperature sensors.

Samples for the investigation are received by the physical vapor deposition of the presynthesized material on the flexible substrates of micamuscovite. The measurement of the thermoelectric parameters of generators was realized at the room temperature on the developed specialized device for impedance spectroscopy of thermoelectric modules. The dimension of p- and n-type legs is 10 mm (length), 2.5 mm (width) with thickness $1-6\mu m$. The generators consist of 3 and 7 p/n couples.

The power of the thermoelectric module is determined by thermoelectric figure of merit ZT. In our latest work it was investigated that thin films based on compounds $Pb_{14}Sn_4Ag_2Te_{20}$ have the highest thermoelectric figure of merit compared to other similar chemical composition [1]. Therefore, films based on $Pb_{14}Sn_4Ag_2Te_{20}$ were used as p-legs and films based on PbTe:Sb were used as n-legs.

The frequency dependences of the impedance for the obtained generators were measured. For the analysis of the received spectra the electrothermal model which allows to receive not only electric but also thermal characteristics of the thermoelectric energy converter is taken as a basis. An investigated modules ZT was in in the range of 1–1.5, which is sufficient to charge the battery of the electronic device. Besides, for the safety, the generator must be in an insulated housing. Considering all the advantages and disadvantages thin film thermoelectric generators based on doped PbTe compounds are promising for use as power sources for micro-size devices.

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Conductivity of polymer films formed by PEO-containing intramolecular polycomplexes

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During the last few decades solid polymer electrolytes (SPEs) have attracted increasing attention due to their possible application in most energy storage/conversion devices. For these devices a non-corrosive, high conductive, electrochemically and chemically stable, low cost electrolyte is very important. The solid solvent-free polymer electrolyte based on amorphous polymer materials could be the best for these purposes.

Among the available polymer matrix of the SPEs, poly(ethylene oxide), PEO, and its derivatives are the most wide studied. However, the high crystallinity of PEO leads to low ion conductivity and inferior Li^+ transference numbers (0.2–0.3) at room temperature, which affects the high rate capability of LBs.

In the present work, we investigated diblock copolymers (DBCs) comprising chemically complementary poly(ethylene oxide)/polyacrylamide which form intramolecular polycomplexes (IntraPCs) and due to this allow to reduce PEO crystallization. We also estimate the influence of humidity on the main dielectric properties of DBC films and examined the DBC partially hydrolyzed derivatives as possible ion-conducting membranes.

Three diblock copolymer samples comprising PEO blocks with variable block length ($Mn_{PEO}=0.75\cdot10^4$, $2\cdot10^4$ and $5\cdot10^4$ kDa) were synthesized and used for this purpose.

The molecular parameters of obtained DBCs are determined by the ¹H NMR spectroscopy. The dielectric characteristics of the studied systems was investigated at 20°C as a function of water content and PEO block length in the frequency range 10^2 - 10^5 Hz using a dielectric spectroscope developed on the basis of the AC bridge P5083 and a three-electrode cell . The water absorption of DBC films was studied at the relative humidities (33%, 65%, 81% and 98%) by gravimetry.

It is noticed that ionic conductivity of DBC membranes does not depend significantly on the length of PEO block and reaches $2.5 \cdot 10^{-10}$ S·cm⁻¹. The introduction of additional ionogenic groups -COOH in polyethylene oxide/poly(acrylamide-*co*-acrylic) acid chains has a positive effect on the conductive characteristics of copolymer membranes and increase the conductivity up to $2.6 \cdot 10^{-9}$ S·cm⁻¹. A significant increase in the ionic conductivity of the copolymer films occurs with increase in adsorbed water and reaches its maximum value $6.6 \cdot 10^{-5}$ S·cm⁻¹.

CdTe / CdS solar modules

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Thin-film solar cells based on cadmium telluride are the basis of that fastmoving technology that has a significant commercial impact on solar energy production. CdTe thin film modules have demonstrated long-term stability, competitiveness and continue to attract investment on an industrial scale.

At the beginning of the XXI century. it was possible to reach a compromise acceptable for production between the two main criteria for the solar module - sufficient efficiency of photovoltaic conversion and cheap products. This was made possible by the development of a number of relatively simple and well-controlled methods for applying thin layers of CdTe and CdS of large area, which are easy to introduce into large-scale production: closed sublimation, chemical vapor deposition, chemical and chemical. The difficulty due to the discrepancy between the parameters of the CdTe and CdS crystal lattices (~ 5%) is largely overcome by the simple temperature treatment of the already fabricated CdTe / CdS structure. It is assumed that the S and Te atoms are mutually substituted, and a $CdTe_{1-x}S_x$ transition layer is formed with a reduced density of states at the interface between CdTe and CdS, which can negatively affect the efficiency of solar cells [1].

The installed modules are well protected, which serves both to protect the cells from environmental influences and to protect semiconductor materials from mechanical damage. By recycling the modules at the end of their service life in the same way as metal products, almost all the cadmium in the module can be recycled at a cost of about 5 cents / W. Because the amount of cadmium used in CdTe thin film modules is quite small, thin film CdTe technology is a minor environmental issue. A 1 m² CdTe module producing about 100 watts using a CdTe layer less than 2 μ m thick contains less than 10 g of cadmium, or about as much as a single flashlight nickel-cadmium battery [2].

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CdTe thin film heterostructures in solar energy

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One of the advantages of CdTe-based semiconductors compared to Si is their more efficient absorption of optical radiation, which allows the production of cheaper thin-film SEs. Moreover, the average efficiency η of heterostructures (HS) of n-CdS/p-CdTe at 300 K under lighting conditions AM1.5 is ~ 16%, which is almost twice less than the theoretical value.

It is believed that one of the reasons for this is the short lifetime τ_s of nonbasic carriers, which causes a high rate of recombination υ_s at the interface between the components of the HS and the grains of the polycrystalline CdTe film. In this regard, a decrease in υ_s (increase in τ_s) should lead to an improvement in the basic parameters of SE namely short-circuit current J_{sc} and no-load voltage V_{oc} . This is confirmed experimentally by the authors, who observed an increase V_{oc} from 0.84 to 0.93 V when replacing the polycrystalline CdTe film with a single-crystal substrate in heterostructural SE n-CdS/p-CdTe. Low values of J_{sc} , and ultimately the efficiency of these samples, due to the high resistance of fairly thick base substrates of p-CdTe, the concentration of free



Fig. 1. Dependences of J_{sc} and V_{oc} for surface-barrier diodes on CdTe:O substrate on the flux density of solar energy radiation.

holes in which at 300 K does not exceed 7 10^{15} cm⁻³. And the improvement of the structural perfection of the photoactive layer of p-CdTe in thin film SE n-CdS / p-CdTe allowed to raise η to ~ 21%, although V_{oc} increased by only 0.03V [1].

The increase in efficiency in this case is associated with an increase in J_{sc} due to a sharp decrease in the series resistance of the HS, which is determined by a thin layer of p-CdTe. The short-circuit current J_{sc} is a linear function of the light level L when it changes within more than four orders of magnitude. The no-load voltage V_{oc} is proportional to lgL at low light levels and tends to saturation at high, Fig. 1.

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RF Magnetron Deposition of ZnO Films on Silicon: Electrical Properties of ZnO/Si Heterostructures

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ZnO films are considered now as a promising electron-selective material for solar cell applications due to unique combination of optical transparency and sufficiently high electrical conductivity. ZnO polycrystalline films exhibit commonly *n*-type conductivity due to structural defects as vacancies, interstitials and antisites. Additional increase in *n*-type doping can be achieved by introducing extrinsic dopants (like aluminum, gallium or hydrogen) into working gas during deposition.

Zinc oxide films were deposited on standard n- and p-type silicon wafers by RF (13.56 MHz) magnetron sputtering. The compacted ZnO powder was used as a sputtering target. During the deposition process into the Ar carrier gas some amount of hydrogen or methane was added to provide additional electron doping of the films. Electrical measurements were done on Ni circular dots (1 mm diameter) created by magnetron deposition through the mask. The samples with addition of 5, 10 and 20% of hydrogen and of 5, 10 and 20% of methane into Ar gas were studied.

At room temperature current-voltage (*I-V*) characteristics of Ni/ZnO/Si structures show weak rectifying behavior with forward branch at V>0 for *n*-Si and at V<0 for *p*-Si. As temperature is lowering down to 150 K, the rectification ratio for structures on *p*-Si increases substantially to 10^3-10^4 due to reduction of reverse currents. This effect is more pronounced for structures with higher content of hydrogen-containing component. The forward currents is higher in samples with higher concentration of H₂ or CH₄, which confirms that hydrogen is being built-in into the ZnO film and acts as *n*-type dopant.

The detailed consideration of I-V and C-V characteristics show that the interface layer between ZnO and silicon (this can be a thin silicon oxide layer) has a high concentration of fixed negative charge. This charge can be caused by charging of a high density of interface states and induces two charge space regions form both sides of the interface.

We have checked also the effect of RF plasma annealing (1.5 W/cm², 10 min.) on the parameters of these structures. It was found that for the structures on *p*-type silicon the rectification ratio improved essentially.

Characteristics of solar cells based on PEDOT:PSS/AgNPs/SWCNT/Si heterostructures

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Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) is a leading p-type organic polymer mixture widely used to create photosensitive organic/inorganic heterostructures. Its performance can be improved by adding Ag metal nanoparticles [1], carbon nanotubes [2] or their mixture [3] to the polymer layer (PEDOT:PSS).

Carbon nanotubes were deposited on the *n*-Si (100) phosphorus-doped substrates by their immersion into the colloid solution of SWCNT in dimethylformamide. The deposition time was 1 minute. The thickness of the nanotube layer varied depending on the number of immersions. Then the organic conductive layer PEDOT:PSS was deposited on Si wafers by spin-coating at rotation speed ω =3000 RPM, time 10-30 s. These films were annealed at 130-170°C in air for 5 min. The deposition of silver nanoparticles was carried out by photoinduced chemical deposition method from an aqueous solution of AgNO₃:HF:H₂O for 10 s.

The thickness of the films and their optical properties were obtained from spectroscopic ellipsometric investigations (SE-2000, Semilab) in the spectral range of 0.6-5 eV. The optical properties of composite films have been modeled as a sum of Drude, Cauchy and Lorentz components. Electrical conductivity of the films was measured using a 4-probe method. Silver nanoparticles in composite increase the light absorption coefficient of the composite mostly in the short-wavelength region of the silicon photosensitivity spectrum.

The dark direct and light current-voltage characteristics of the developed solar cells were investigated. Improvements in the parameters of current-voltage characteristics (primarily in the short circuit current I_{sc}) are observed with an introduction of nanotubes and silver nanoparticles into PEDOT:PSS composite.

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Activation processes in cadmium telluride films

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The investigations are devoted to the study of the influence of physical and technological conditions of "chloride" treatment on the crystal structure of the base layers of cadmium telluride and the efficiency of film solar cells based on them.

It is established that when carrying out solid-state "chloride" treatment of base layers of cadmium telluride, which are obtained by thermal vacuum evaporation, the concentration of copper in the cadmium chloride charge and the deposition rate of cadmium chloride layers are significant technological factors influencing the efficiency, because the presence of copper leads to additional doping of the base layers, and excessive deposition rate leads to the appearance of electric shunts in the area of the separating barrier. At the same time, modes of "chloride" treatment were identified, which allow to form instrument structures with an efficiency of up to 10%.

It was found that gas-phase "chloride" treatment of cadmium telluride layers obtained by sublimation in a closed volume is more efficient than solidstate, which is due to the negative effect of inflated values of diode saturation current density and series resistance and is associated with experimentally established higher lower macroform. layers and less intense interfacial interaction of CdTe-CdCl₂. The modes of "chloride" treatment of cadmium telluride layers obtained by sublimation in a closed volume, which is carried out by annealing in vapors of cadmium chloride and provides the formation of solar cells with an efficiency of 12.8%.

It has been shown that when annealing in freon the layers of cadmium telluride obtained by sublimation in a closed volume at a temperature of 400 °C for 30 minutes, solar cells based on them show an increase in efficiency to 11.7%. Further exposure of these instrument structures when illuminated in the AM1.5 mode leads to an increase in efficiency to 12.4%. When annealing the layers of cadmium telluride in freon obtained by thermal vacuum evaporation, the greatest increase in the efficiency of solar cells based on them up to 7.2% is observed at an annealing temperature of 450 °C, if it lasts 25 minutes.

It is experimentally proved that the "chloride" treatment carried out by annealing the base layers of cadmium telluride, obtained by sublimation in a closed volume, in vapors of cadmium chloride, in comparison with annealing in Freon, allows to obtain greater efficiency of solar cells based on them due to lower the value of the series electropore, which is due to the more intensive generation of electrically active intrinsic point defects, because during the annealing in freon interfacial interaction of chloride and cadmium telluride is preceded by the stage of formation of cadmium chloride.

Intercalation of Li Atoms in TaSe₂ Film's Anode with LiClO₄/PEO Polymer Electrolyte: First Principles Calculation

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A promising source of electrical energy storage is $TaSe_2$ films, which have a layered structure. This structure consists of repeating two-dimensional sandwiches arranged as Se-Ta-Se, which are covalently linked. Each such Se-Ta-Se monolayer is bound to the next monolayer by Van der Waals forces. Small ions or molecules can be intercalated in the interlayer space, which allows the use of such a material as the anode of lithium-ion batteries [1, 2]. To improve the anode properties of lithium-ion batteries based on transition metal dichalcogenides, they are supplemented with an ionic liquid, for example, LiClO₄/PEO polymer electrolyte [4]. Such polymer electrolytes are particular interest due to the formation of lithium-polymer complexes with high mobility of lithium ions.

Using the methods of electron density functional and pseudopotential from the first principles, the total energy, energy reliefs and migration barriers of Li atoms in the interlayer of 2H-TaSe₂ monolayer, spatial distributions of valence electron density and their cross sections were calculated.

An increase in the value of the energy barrier during the migration of Li atoms with an increase in the number of intercalated Li atoms, which filled the interlayer space, was observed for all studied anode materials except for $TaSe_2$ with molecules of PEO polymer electrolyte. It was found that the values of effective electric charges of Se atoms in $TaSe_2$ film with composite additives are different and depend on the position of the Se atom relative to the polymer molecules, the position of the intercalated Li atom relative to the Se atom and the layer filling with Li atoms. In the anode of the battery based on $TaSe_2$ film with LiClO₄/PEO polymer electrolyte uniformity of electric charges on Se atoms which limit the layer in which Li atoms move is observed. This fact manifests itself in the energy consumption of migratory movements of Li atoms in the anode, namely, it becomes monotonous.

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Novel proton conductive polymer/inorganic membranes for fuel cell application

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Fuel cells are considered to be a promising technology for power applications owing to their high efficiencies and low emissions. Membrane is the core component of the polymer electrolyte fuel cell (PEMFC). That is why; high-performance membrane material is a one of major challenge for the effective PEMFC operation.

The hybrid polymer/inorganic proton conductive membrane based on poly(2-acrylamido-2-propanesulfonic acid-co-acrylic acid-co-acrylonitrile) with added sol-gel system containing tetraethoxysilane and 3-methacryloxypropyl-trimethoxysilane as precursors has been synthesized by *in situ* photopolymerization of acrylate groups and inorganic condensation of silanol groups. The N,N'-methylene(bis)acrylamide was used as a cross-linker agent.



Fig. 1. a) Cross-sectional SEM image and b) proton conductivity (PC) of the membrane PA/SGM5 at different temperatures

The internal structure of the membrane cross-section was evaluated using SEM. The corresponding image are shown in Fig. 1a) demonstrating the formation of silica domains in polymeric matrix. Fig. 1b) shows the result of the membrane proton conductivity (PC) measurements at 95% RH obtained during fuel cell operating. PC of the membrane sufficiently depends on temperature and values decreased with increasing of the temperature. Results of the synthesized membrane PC reaches to the Nafin 117® ($5.33*10^{-2}$ S/cm, T=50°C).

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Pulsed laser grown of topological insulator Bi₂Te₃ and Bi₂Se₃ thin films

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Studies of three-dimensional topological insulators (TI), such as Bi_2Te_3 , Bi_2Se_3 , have been intensive over the last decade. This is due to their unique physical properties and potential applications for spintronics and quantum computing. These materials express the effects of a strong spin-orbit bond (SOC), which occurs as a result of the presence of heavy elements Bi, Se and Te. Also, semiconductor compounds of type V_2VI_3 , due to the high coefficient of thermoelectric conversion Z, are known as materials for thermoelectric devices encourages to study not only the properties of massive samples, but also the properties of thin films of these materials. In particular, the compound Bi_2Te_3 and Bi_2Se_3 is currently the best thermoelectric material, especially when using ultrathin films.

In this work, thin Bi₂Te₃ films of electronic and hole conductivity obtained by pulsed laser deposition in vacuum were investigated. Alloys for the manufacture of targets were synthesized from a mixture of elements Bi, Te with the addition of alloying impurities. The targets were evaporated using a Nd: YAG laser on Al₂O₃ and Si substrates heated to 200–300 ° C. Laser parameters: ≈ 1064 nm; Emax ≈ 0.4 J; $\Delta \tau \approx 10$ ns, pulse repetition frequency f ≈ 1 Hz. Films with a mosaic single-crystal structure about 1 µm thick were obtained. The constants of crystal lattices a and c of rhombohedral structure are determined.

The study of electrical and thermophysical properties of the obtained films was carried out. Measurements of temperature dependences of the resistivity of the obtained films were performed in the temperature range of 80-300 K. Thermophysical characteristics, in particular, temperature dependences of the Seebeck coefficient, were also studied. The relationship between the structure of thin films and their electro- and thermophysical properties is established.

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SCAPS modelling of the photovoltaic properties of the Copper dopind of CdTe films

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CdTe is a direct-band semiconductor that can have both n-type and p-type conductivity, depending on the use of appropriate alloying impurities. Therefore, controlled doping of these materials with p and n-type of carriers we can significantly improve the efficiency of PV-modules based on them [3].

Fig. 1 shows the SCAPS solar cell definition panel, where specific parameters for each layer can be set. The conversion efficiency of solar radiation into photoelectric energy is determined by the width of the band gap of the studied heterostructure. SCAPS simulation tool allows to build appropriate band diagrams.



Fig. 1. SCAPS definition panel.

The deposition technology is developed and the influence of copper impurity concentration on the optical properties of CdTe thin films is studied. To obtain thin films, the method of open evaporation in vacuum is used, which ensures the purity of the film due to the high vacuum [4]. In [1] show that the band gap decreases slightly with increasing concentration of the alloying impurity (Eg₁ = 1.50 eV (for 1% Cu), Eg₂ = 1.48 eV (for 2% Cu), Eg₃ = 1.45 eV (for 3% Cu)), however, a high absorption coefficient is observed in the film. Therefore, thin CdTe films doped with 3% Cu will be suitable for the p-layer of a highly efficient p-n solar cell, based on CdTe.

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$\begin{array}{c} Resolving \ power \ of \ optical \ recording \ image \ on \ nanostructures \ metal-\\ dielectric-Cd_{1-x}Zn_xTe \end{array}$

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Semiconductors CdTe, ZnTe and solid solutions based on them $(Cd_{1-x}Zn_xTe)$ are of great interest from a technological point of view due to their use in optoelectronics. This material is suitable for photorefraction and elements for optical recording media on metal-dielectric-Cd_{1-x}Zn_xTe nanostructures. The presence of electrically active centers in such single crystals due to the thermodynamic features of their growing leads to a violation of the symmetry of chemical bonds of which leads to a decrease in the recording detector charge.

Equally important is the value of dark current, which is determined by the concentration of electrically active centers and is responsible for reducing the resolution. One of the methods to reduce the level of defects and improve the effect of image recording there is hydrogen passivation. Such passivation was technologically carried out as a result of hydrogen implantation or crystal treatment in the hydrogen atmosphere discharge [1].

In this paper obtained the expression for the resolution of optical-recording nanostructures metal-dielectric-semiconductor $Cd_{1-x}Zn_xTe$ ($0 \le x \le 1$). For the non-passivated semiconductor material $Cd_{0.8}Zn_{0.2}Te$ the resolution is $R_1 = 6682$, and for the passivated one in the hydrogen atmosphere $R_2 = 17423 R_2/R_1 = 2.6$, i.e. it is possible to read separately two recording signals with a minimum wavelength interval of 150 *nm* and 57 *nm* respectively.

The resolution of optical image recording on nanostructures metaldielectric-Cd_{1-x}Zn_xTe is also related to the concentration of atomic hydrogen N_H : if this concentration does not exceed the concentration of acceptors, the passivation by atomic hydrogen of electrically active centers leads to increase of resolution, while in the case of $N_H > N_A$ - to reduce it.

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The influence of mercury concentration and temperature on the electrical resistance of Hg modified amorphous films

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In [1] it was shown that the exposure of amorphous Se films in mercury vapor leads to a decrease in their electrical resistance by several orders of magnitude, and the magnitude of change in resistance largely depends on the thickness of the films. The reason, according to authors opinion [2], is the formation of crystalline inclusions of mercury selenide in the mercury-activated amorphous film of selenium. Due to the fact that the rate of mercury evaporation and consequently its concentration in a certain volume is determined by the size of the open area and its temperature, it can be assumed that these parameters will affect the rate of formation of mercury selenide in amorphous selenium film. Accordingly, the electrical properties of the modified films will change.

This abstract presents the results of studies on the effect of mercury concentration and temperature on the electrical resistance of amorphous selenium films.

Studies of the dependences of resistance on the exposure time in mercury vapor were performed in special air-tight boxes on planar structures «Ni layer – Se film - Ni layer» at T = 287-296 K. It is established that there is a latent period, during which resistance of the planar sample remains almost unchanged. Its duration, depending on the concentration of mercury and temperature, is from tens of minutes to several hours. Subsequently, the resistance of planar samples decreases sharply (by 4-6 orders of magnitude). As the temperature and concentration of mercury increase, the duration of the latent period decreases, and the rate of change of resistance increases.

The reason for the sharp decrease in the resistance of planar structures "Ni-film layer Se-Ni layer" during their exposure in mercury vapor is the formation of crystalline inclusions of mercury selenide in the amorphous matrix of selenium, which have high electrical conductivity.

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Influence of nanodots scattering on thermoelectric figure of merit

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Recent decade it was found that thermoelectric materials with significant contribution to scattering at potential barriers, have increased thermal efficiency. This improvement can be considered related to nanoscale inclusions. Better results in terms of increasing thermoelectric efficiency were obtained for nanostructured materials containing quantum wells, barriers, quantum dots. Therefore, the study of thermoelectric nanocrystalline materials has particular interest.

Transfer phenomena for nanocomposites can be described as carriers scattering on the grain potential barrier in combination with phonon scattering. The scattering of electrons on the barrier depends to the energy, which leads to the effect of energy filtration, which increases the Seebeck coefficient. The combination of this mechanism with the scattering of phonons on the nanoinclusions causes a significant increase of the thermoelectric figure of merit. Calculations performed for some materials have been shown that superlattices or quantum dots leads to an increase of the thermal efficiency. There were considered spherical, ellipsoidal and other forms of nanoinclusion, which are randomly distributed in the bulk semiconductor material. Such evaluations were performed for nanoinclusions in InGaAs, Si, PbTe and other materials.

In this paper the theoretical model and numerical calculations of the thermoelectric properties of semiconductor materials which containing nanoparticles described by the Gaussian potential with different values of its parameters are shown. This type of potential often is used to describe the properties of quantum dots. The transmittance for all values of the potential parameters was obtained numerically using by applying the tridiagonal matrix algorithm. The results of numerical calculations were used for computer modeling of the Seebeck coefficient and lattice thermal conductivity. The potential parameters are selected with the characteristic dimensions of the nanoinclusions in range 5 - 10 nm. The results of the calculations showed an increasing of the Seebeck coefficient and significant decrease of the lattice thermal conductivity at temperatures below room temperature.



POSTER REPORTS

Session 7 Innovative methods for teaching



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General provisions for elective chemistry courses for students within the scope of Bologna process

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In comparison with core subjects, elective courses, have better context variability, and also strengthen practical, research, and experimental parts of profile studies. They have non-standard character and take into account regional conditions. They will help to eliminate contradictions between educational needs of young people and existing traditional "range" of school subjects.

Special features of elective courses include necessity for pupils to choose some of specific courses (5-6 and more) and to attend them. Such choice places pupil in situation of personal professional self-determination and structuring of individual career.

Elective courses may have several functions including the following: 1) learning the main problems within chosen knowledge field; 2) learning the main profile subjects at a good level because of enrichment of core course with additional information which makes knowledges of the main subjects wider and dipper; 3) focus on behavioral aspects of course content, improvement of perceptional, practical, and research activities skills; 4) ensuring of effective intra-profile majoring by means of wider usage of subjects interrelations.

The aim of elective courses is pupils' focusing on education individualization and socialization, training them for comprehended and responsible choice of the future professional activity sphere. In order to specialize learning, elective courses *subjects* and *content* have to fit the following requirements:

a) assistance in pupils socialization and adaptation and in their comprehensive professional self-determination;

b) presence of social and individual meaning, providing possibility for profound specialization and for choice of individual path for training;

c) assistance in learning basic and professional educational subjects, and also ensuring conditions presence for intra-profile specialization of education;

d) essential developmental and educational potential;

e) assistance in integral world view formation;

f) assistance in development of educational, intellectual, and professional skills and experience.

General requirements for chemistry elective courses for pupils in the context of Bologna process

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Elective courses program has to include explanatory note, educational subjects plan with developed content characteristic, literature listing, and attachments. Educational subjects plan (see the table) should include topics titles, time amount needed for these topics learning (lectures and practice hours), studies form, educational materials to be developed by pupils during their cognitive and research activities: notes, theses, experimental results, historical analyses, poems, narrations, diagrams, pictures, embroidering, models etc. At the end of the plan the following have to be presented: detailed characteristic of every topic and brief annotations of laboratory experiments (instructions for their carrying out, necessary equipment). Contents should include not only knowledges to be obtained by pupils, but also other components: educational creative pupils' activities experience (known methods), emotional and evaluational relationship experience. Mastering these types of experience, and also adopting common knowledges and skills, give possibility to form students' ability for culture-adequate activities.

No.	Elective courses function	Programs titles	
		10 th class	11 th class
1	Widening the scope of existing profile chemistry courses	Qualitative analysis fundamentals (analytical chemistry)	Colloid chemistry fundamentals
2	Intra-profile specialization	General ecology (environment pollution with inorganic substances)	General ecology (environment pollution with organic substances)
3	Practical orientation	Modern materials in inorganic chemistry (ultrapure, binary etc.)	Modern materials in organic chemistry (plastics, fibres, resins, composite materials)
4	Professional orientation	Chemistry in medicine	Chemistry in agriculture
5	Content integration	Electrochemistry fundamentals (based on chemistry and physics)	Biochemistry fundamentals
6	Content development	Redox-reactions chemistry	Chemical processes thermodynamics

Table. Elective courses in chemistry

Cloud technologies in the teaching of chemical disciplines

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Today requires new approaches to the educational process, new methods, forms of presentation of educational information. In particular, new approaches are needed in the teaching of chemical disciplines. One such approach is the use of cloud technologies. The use of cloud technologies in the teaching of chemical disciplines allows to intensify the educational process, accelerate the transfer of knowledge and experience, as well as improve the quality of teaching and education. Without cloud technologies it is impossible to imagine the educational process in a blended learning environment.

Distance learning software plays an important role in blended learning. Today, every educational institution has the opportunity to choose the most convenient learning platform for him. In IFNMU there is a licensed internal portal based on cloud technologies Microsoft Office 365. And also organized:

1. Email Live Outlook.

2. File storage SkyDrive.

3. Office Live – Word, Excel, PowerPoint, Teams, OneNote.

4. Workspace for collaboration: shared calendar, web conferencing, instant messaging, desktop sharing, storage of shared files and the ability to collaborate on documents.

The site contains all the necessary materials for training, including presentations, videos. It is known that the best absorbed is what is perceived by several senses. This feature affects the fact that Internet technology can provide: demonstrativeness, fragmentation, methodological invariance, conciseness, heuristics, independence. The construction of a virtual chemical laboratory allows the teacher through the use of visual models and interactive animation to more easily explain the essence of complex phenomena and processes, to demonstrate "virtual" experiments and experiments without the necessary laboratory equipment. The set of options of the virtual chemical laboratory allows to study quantitative and qualitative characteristics of processes and the phenomena of environment, models of the difficult technical devices and the equipment used in scientific researches and technological processes.

Thus, using the "cloud" of the university, students will gain access to many programs and opportunities. Cloud technologies greatly simplify data storage and use of materials. An important advantage of this technology is the involvement of students in the main direction of development of network technologies in modern society. In the process of work, students are instilled with a culture of independent work with network resources at a fairly high level.

Innovations in teaching of fundamental sciences

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Teaching physics in high school faces many challenges. First of all, the variety of physics courses confined to a limited time frame may seem to the students detached from real life and not needed in further engineering. However, studying the whole physics course, rather than its sections, allows one to form a holistic picture of the world and comprehend the basic principles of Nature. This understanding cannot be achieved immediately; it comes gradually over time and with the acquisition of professional experience by a specialist. Therefore, the ultimate goal of the university is to encourage students to study fundamental disciplines.

Experience shows that the traditional approach to higher education does not compete with the practical needs of today's rapidly evolving world. The accumulation of fundamental knowledge without seeing their direct and rapid application creates a lack of motivation for learning for some students. Therefore, to introduce changes in learning, it is necessary to train motivational levers for learning. The implementation of such a task is possible with the use of innovative methods in teaching. Such practices have a dual function. They allow to accumulate knowledge in a particular subject and develop other vital skills for the future professional. It is known that only 15% of career success depends on "hard skills," while the remaining 85% of career success is determined by "soft skills." The development of soft skills is an essential requirement for learning.

Mastering the students' soft skills will help them understand that learning does not end after university but continues the entire life. Education is a continuous process, the main part of which belongs to self-education. So the ability to learn throughout life is the first requirement that the university has to engrave in students' mind. And this will be facilitated by the ability to work in a team, find different ways to solve engineering or scientific problems, not give up before obstacles, have an emotional state, and be able to negotiate and compromise. The development of such "soft skills" should be part of compulsory education.

In present work, an original scheme of calculation and graphic work by students that allows developing comprehensively, along with solid skills, soft skills, which are vital for further career growth of future professionals, is proposed.

Professional risks in the process of electromedical equipment exploitation

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Numerous experimental studies show that the use of electromedical equipment helps to maintain, strengthen and restore human health. The analysis of working conditions of medical staff is based on a differentiated determination of the influence of individual factors of the working environment. At simultaneous action of several harmful factors it is necessary to analyze their integral action.

In modern conditions, it is important to minimize both professional risks and the risks caused by the action of harmful and dangerous factors on the patient's body. Electromedical equipment uses electromagnetic radiation (EMR). Almost any system that has energy, chemical or biological components is dangerous. The danger can be potential or real. Potential danger becomes real if three conditions are met: the danger actually exists, the person is in the danger zone, the person does not have sufficiently effective means of protection. All technical equipment for treatment and other means of rehabilitation must be safe, high quality and easy in operation. In addition, it is necessary to take into account possible changes in the technical characteristics of the equipment over time. In order to prevent injuries and deteriorate health of patients and medical staff, each workplace provides an instruction, which sets out the general and qualification requirements, duties, rights, responsibilities.

Radiation exposure, even in small doses, can have a negative effect on health. This is often due to stochastic effects. Safety measures require a set of different protective measures, depending on the specific working conditions with EMR sources and their type. In many medical devices, the image is sent to the doctor's computer monitor, where he can examine it without exposing the patient to additional radiation.

Nowadays, it cannot be said that the effects of EMR, even with levels below the limit values of national norms, are potentially completely safe for health.

To predict the degree of EMR damage of tissue, it is necessary to build mathematical models of damage. In the process of creating these models, it is necessary to take into account the nature of the distribution of electromagnetic energy around the source and the peculiarities of irradiation of biological tissue.

Generalization and systematization of knowledge of the high school students' about light diffraction

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Improving the educational process requires intensive work on mastering the content of educational programs, using the achievements of pedagogical science in the educational process. The introduction of lessons of generalization and systematization of knowledge in the educational process contributes to the comprehensive development of independence and initiative of students, acquainting them with research methods and logic of scientific thinking, the laws of cognition, the formation of a physical picture of the world.

To clarify the phenomenon of light diffraction, generalization and systematization of high school students' knowledge on this topic, it is advisable to use sign-symbolic visualization [1]. The interaction of the teacher with the students and students among themselves and the increasing motivation of pupils to study physics are important in this process [2,3]. During the dialogue with the class, the student-teacher-student interaction, and discussion each cell of the block diagram is filled. At this stage of generalization and systematization of students' knowledge, an important factor is not only the use of formulas but also graphs, drawings, and textual information.

In this work, we present the results of research on the use of block diagrams, tables and figures in the generalization and systematization of high school students' knowledge of the wave properties of light, in particular diffraction.

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