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Аннотации на английском языке

Review

Review article
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Graphitic carbon nitride: properties and applications in gas sensing. Review

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Abstract
Purpose: Nowadays gas sensors are of great interest for disease detection and assessment of treatment efficacy based on exhaled breath analysis. One of the promising materials for gas sensors are composites of graphitic carbon nitride with metal oxides.
Experimental: The article considers the basic properties of g-C_3N_4 and provides a review of methods that can be effective for obtaining its composites with metal oxides.
Conclusions: The study presents the mechanism of interaction of g-C_3N_4 with gases of different nature. In addition, it gives some examples of sensors based on composites of g-C_3N_4 with metal oxides.

Keywords: Graphitic carbon nitride, Gas sensing, Nanocomposites
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Review article
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Advanced methods for preparing especially pure glasses based on germanium and gallium chalcogenides. Part 2. Synthesis using chemical transport reactions. Review

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Abstract
Purpose: The second part of the review presents the results of preparing especially pure glasses based on germanium and gallium chalcogenides with chemical transport reactions.
Experimental part: Deep purification and vacuum loading of metallic gallium, gallium(III) telluride and rare-earth elements (REE) using gallium(III) iodide as a transport agent made it possible to reduce the content of hydrogen, oxygen impurities and heterogeneous inclusions in glasses by 1–2 orders of magnitude compared to tradition direct glass synthesis. We have theoretically justified and experimentally confirmed the high efficiency of REEs as getters for binding and subsequent removal of oxygen impurities from the chalcogenide melt.
Conclusions: The key result achieved by reducing the impurity content is mid-infrared (IR) laser generation in bulk samples of REE-doped chalcogenide glasses and in optical fibers based on them, which was previously not possible in these materials.

Keywords: Chalcogenide glasses; Especially pure substances; Optical materials; Synthesis; Chemical transport reactions; Laser generation
Funding: The research was carried out with the financial support of the national project "Science and Universities" at the laboratory "High-purity chalcogenide glasses for mid-IR photonics", state order FFSR-2024-0001 and the Research and Education Centre of the Nizhny Novgorod region within the framework "Technoplatform 2035" project.
For citation: Velmuzhov A. P., Sukhanov M. V., Tyurina E. A., Shiryaev V. S. Advanced methods for preparing especially pure glasses based on germanium and gallium chalcogenides. Part 2. Synthesis using chemical transport reactions. Review. *Condensed Matter and Interphases*. 2025;27(2): 190–202. https://doi.org/10.17308/kcmf.2025.27/12770

Original articles

Research article
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On the mechanism of recrystallization of bismuth chalcogenides during photonic treatment with incoherent radiation

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Abstract
Purpose: The aim of this work is to reveal the nature and systematize the mechanisms of gradient structure formation in the surface layer of bismuth chalcogenide during photon treatment with incoherent radiation from xenon lamps.
Experimental: Semiconductor thermoelectric branches based on Bi_2Te_3–Bi_2Se_3 solid solutions have been investigated by transmission

electron microscopy, X-ray diffractometry, and photometry methods. The nature of nanostructuring and formation of gradient layer in the surface region of $Bi_2Te_{3-x}Se_x$ thermoelectric at photon treatment by incoherent radiation of xenon lamps is considered.
Conclusions: It is shown that these processes can be caused by a sequence of independent processes: growth of free electron concentration, decrease of defect formation threshold, localization in skin layer of high temperature gradient, generation and propagation of sonic phonons, collecting and secondary recrystallization, formation of nanocrystalline phase in Bi-Te-Se system.
Keywords: Photon treatment, Recrystallization, Electron microscopic micrograph, X-ray diffractometry, Nanostructured layer, Lattice defects, Bismuth chalcogenides
For citation: Belonogov E. K., Kushchev S. B., Serikov D. V., Soldatenko S. A., Turaeva T. L. On the mechanism of recrystallization of bismuth chalcogenides during photonic treatment with incoherent radiation. *Condensed Matter and Interphases*. 2025;27(2): 203–210. https://doi.org/10.17308/kcmf.2025.27/12764

Research article
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Investigation of the possibility of ice film 0 formation on the dielectric surface in a microwave resonator
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Abstract
Purpose: The possibility of detecting ice 0 by deposition of water vapor on quartz glass dielectric plates placed in the cavity of a microwave rectangular resonator near the frequency of 2.8 GHz is investigated.
Experimental: Measurements of the characteristics of the resonator filled with air at atmospheric pressure in the temperature range from 5 to –140 °C have been performed. Variations of the transmittance power of the resonator at the resonance frequency and its quality factor of fit were found with their characteristic change at a temperature of –23 °C. This temperature corresponds to the formation of ice 0 from supercooled water. It is assumed that in the experiment, films of ice 0 are detected in the response of the resonator to the temperature change in the investigated interval.
Conclusions: This result is of interest due to the possible influence of water vapor condensation on the functioning of a variety of technical devices in terrestrial conditions when ice 0 is formed.
Keywords: Ice 0, Conductive films, Microwave range, Resonator measurements
For citation: Bordonskiy G. S., Kazantsev V. A., Kozlov A. K. Investigation of the possibility of ice film 0 formation on the dielectric surface in a microwave resonator. *Condensed Matter and Interphases*. 2025;27(2): 211–216. https://doi.org/10.17308/kcmf.2025.27/12765

Research article
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Self-assembly of cationic polymers in mixed polymer-lipid monolayers at the liquid-air interface
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Abstract
Purpose: The self-assembly of cationic polymers at the liquid-air interface is the most important process for the design of new targeted drug delivery systems, including lipid-polymer hybrid nanoparticles.
We studied the self-assembly of cationic pH-sensitive polymers at the liquid-air interface in mixed Langmuir polymer-lipid monolayers of cholesterol with Lipoid S100.
Experimental: We used synthetic approaches to the synthesis of ionene polymer and studied its physicochemical properties by NMR, IR, HPLC, and gel permeation chromatography. The surface behavior and states of polymer monolayers and their mixtures with lipids (compressibility and molecular area) at the liquid-air interface were examined using the Langmuir-Blodgett technique. The resulting lipoplexes were studied by dynamic light scattering (average weight diameter and zeta potential).
Conclusions: High stability of lipid-polymer nanoparticles was achieved for compositions of mixed monolayers with the compressibility modulus (Cs^{-1}) of at least 50 mN/m. In this case. the particle sizes were in the range from 32 to 73 nm and the zeta potential values for non-quaternized cationic polymers were strongly negative (from –15 to –45 mV), while for the ionene polymers they were significantly positive (from +8 to +49 mV).
Keywords: Self-assembly at interfaces, Polymer-lipid nanoparticles, Langmuir monolayers, Ionene polymers
Funding: The study was supported by the Russian Science Foundation (grant No. 22-73-10220).
For citation: Kamorin D. M., Simagin A. S., Kazantsev O. A., Slivkin A. I., Zamyshlyayeva O. G., Emasheva A. A., Melnikova N. B. Self-assembly of cationic polymers in mixed polymer-lipid monolayers at the liquid-air interface. *Condensed Matter and Interphases.* 2025;27(2): 217–225. https://doi.org/ 10.17308/kcmf.2025.27/12863

Research article
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The potential corrosion inhibition properties of acetyl benzoic acid derivatives with substituted alkali metals (Na, K, Li): DFT approach
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Abstract
Purpose: Inhibitors of corrosion shield metals from corroding. Such chemicals may be added to a corrosive environment to either halt or slow down metal corrosion. The molecular structure of 3-acetyl benzoic acid (3ABA) $C_9H_8O_3$ consists of planar molecules. These molecules aggregate by centrosymmetric hydrogen-bond pairing of ordered carboxyl groups. The novelty of the research and its primary objective was to perform a theoretical computational study on derivatives of 3ABA-M (Metal), where M molecule is modified by adding lithium (Li), sodium (Na), and potassium (K).
Experimental part: The study was carried out withing the framework of the density functional theory (DFT) at the B3LYP/6-31G+ (d) level in the Gaussian 09W software. It involved geometrical optimization, analyzing spectral properties, electronic transitions, and the energy gap between the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO). The calculated properties included E_{HOMO}, E_{LUMO}, energy band gap (Egap), ionization energy (IE), electron affinity (EA), absolute electronegativity (χ), global hardness (η), and global softness (S).
Conclusions: The chemical reactivity of the studied molecule was investigated by analyzing its molecular electrostatic potential (MEP) and electron localization function (ELF), using the Multiwfn 3.7 software. Consequently, it was concluded that the large energy gap of 3BAB (5.617 eV) and its high hardness (2.809) correlate with a low refractive index, dielectric constant, and low corrosion inhibition, whereas significant molecular softness of 3ABA-Na (2.88 eV^{-1}) is associated with a high refractive index.
Keywords: 3-Acetyl Benzoic Acid, Corrosion Inhibition, DFT, Electron Localized Function, Refractive Index
Acknowledgements: We express our gratitude to the leaders of Department of physics, college of Science & Halabja University.
For citation: Kareem R. O., Hamad O. A. The potential corrosion inhibition properties of acetyl benzoic acid derivatives with substituted alkali metals (Na, K, Li): DFT approach. *Condensed Matter and Interphases.* 2025;27(2): 226–236. https://doi.org/10.17308/kcmf.2025.27/12811

Research article
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DFT analysis: correlation of epinephrine HOMO-LUMO, refractive index, optical electronegativity, and electrical conductivity with Substituted Halogens (F, Cl, Br)
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Abstract
Purpose: Epinephrine (EP) may affect lipid and glucose metabolism in addition to haemodynamic parameters, according to a number of studies. This study's primary goal was to provide a theoretical computer analysis of the EP molecule by including halogens like fluorine (F), chlorine (Cl), and bromine (Br): (EP, EP-Br, EP-Cl, and EP-F).
Experimental part: The Gaussian program was used to obtain the optimal shape of the EP compound, and the DFT/6-311G (d,p) basis set and B3LYP level of theory were employed. Quantum chemistry properties were then analyzed, including the energy gap (E_{HOMO}-E_{LUMO}), reduced density gradient (RDG), density of states (DOS), and molecular electrostatic potential (MEP) on surfaces.
Conclusions: The results showed that the larger refractive index of the EP-F molecule was associated with a higher value of EP-F (0.446 eV^{-1}) molecular softness, while the EP molecule exhibited higher hardness (η) (2.296 eV) and a smaller refractive index. On the other hand, a smaller bandgap for EP-F (4.483 eV) indicated reduced chemical stability, increased electron dispersion, a lower work function (2.40682 eV), and improved electrical conductivity (σ = 1.249). According to our Electron Localized Function (ELF) topological analysis data, the group of H atoms had a red patch around them, indicating an abundance of delocalized electrons.
Keywords: Epinephrine, DFT, Refractive Index, Electron Localized Function (ELF), Electrical Conductivity, Optical Electronegativity
Acknowledgements: We express our gratitude to the leaders of Department of physics, college of Science & Halabja University.
For citation: Kareem R. O. DFT analysis: correlation of epinephrine HOMO-LUMO, refractive index, optical electronegativity, and electrical conductivity with Substituted Halogens (F, Cl, Br). *Condensed Matter and Interphases.* 2025;27(2): 236–. https://doi.org/10.17308/kcmf.2025.27/12811

Research article
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Influence of external influences on the activation of domain walls of ferroelectric perovskites
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Abstract
Purpose: The article aims to establish the regularities of the influence of external influences (thermal and electrical) on the activation of domain walls in oxygen-octahedral-type ferroelectric materials with perovskite structure which have a wide application in electronic devices. One of the problems in this case is the stability of domain walls with respect to external influences. With this in mind, the aim of the paper is to determine the activation energy of irreversible motion of domain walls when switching the polarization of a ferroelectric by electric field in a wide temperature range.
Experimental: The value of the critical energy W_{max} of interaction of ferroelectric domains with an external electric field necessary for irreversible change of the domain structure of a ferroelectric under different thermal conditions is determined. For this purpose, the dielectric hysteresis loops $P(E)$ of samples obtained at different temperatures were analyzed. Ferroelectric materials with oxygen-octahedral

perovskite structure were chosen as objects of study: $BaZrO_3/BaTiO_3$ superlattice, $Pb(Zr_{0.3}Ti_{0.7})O_3$, ceramics $(Pb_{0.96}Sr_{0.04}(Mg_{1/3}Nb_{2/3})_{0.275}(Ni_{1/3}Nb_{2/3})_{0.1}Ti_{0.375}Zr_{0.25}O_3$ and ceramics $Pb_{0.88}Ba_{0.06}Sr_{0.06}(Mg_{1/3}Nb_{2/3})_{0.37}Zr_{0.375}Ti_{0.255}O_3$).
Conclusions: Temperature dependences of the critical energy W_{max} of interaction of ferroelectric domains with an external electric field necessary for irreversible change of the domain structure of a ferroelectric have been determined. The assumption that the energy W_{max} has the meaning of the activation energy of the domain structure of a ferroelectric at switching of polarization by an electric field, necessary for irreversible change of its domain structure, has been substantiated. It is established that the critical energy W_{max} decreases linearly with temperature in a wide temperature range below the Curie point. The obtained results have scientific and practical value, since they allow to determine the conditions of stability of the domain structure of a ferroelectric to external influences and expand the possibilities of application of the Sawyer-Tauer method for determination of activation energies of irreversible change of the domain ferroelectric structure.
Keywords: Ferroelectric perovskites, Domain walls, Dielectric hysteresis loop, Activation energy, Repolarization, Barium zirconate, Barium titanate, Lead zirconate titanate, Lead magnoniobate
Funding: The research is a part of fulfillment of the State assignment of the Ministry of Science and Higher Education of the Russian Federation "Activation mechanisms of phase transitions in ferroelectric materials" (FREU-2023-0001).
For citation: Kuzenko D. V. Influence of external influences on the activation of domain walls of ferroelectric perovskites. *Condensed Matter and Interphases*. 2025;27(2): 251–259. https://doi.org/10.17308/kcmf.2025.27/12864

Research article
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Modeling of Desloratadine release process from alloys with Polyethylene glycol-6000 by Molecular dynamics method
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Abstract
Purpose: Desloratadine is a drug with proven antihistaminic activity, is currently presented on the pharmaceutical market only in dosage forms: tablets, solution and syrup. A significant factor limiting the development of new drugs of desloratadine is its low solubility in water. The actual direction of pharmaceutical technology in this regard is research on creation of dosage forms of desloratadine, aimed at increasing its water solubility. Currently, a promising direction in pharmaceutical technology in the development of drug composition is the use of computer modeling. The use of molecular dynamics modeling method is very relevant in the development of solid dispersions of drugs. The aim of this study was to carry out molecular dynamics modeling of desloratadine release from alloys with polyethylene glycol-6000 (desloratadine: polymer ratio 1:1, 1:2, 1:5) into the dissolution medium.
Experimental: modeling of desloratadine release from alloys with polyethylene glycol-6000 was carried out by molecular dynamics method (Gromacs 2023 program, Amber 99 force field). The van der Waals interaction energies of desloratadine with polyethylene glycol-6000 and with water were calculated; the fraction of desloratadine molecules that lost the bond with polyethylene glycol-6000. It was found that the average energy of interaction of desloratadine with polyethylene glycol -6000 and with water. Polyethylene glycol-6000 decreases as the content of desloratadine in the alloy decreases. Desloratadine in the alloy, while the interaction energy with water increases.
Conclusions: The studies on the release rate of desloratadine from alloys with polyethylene glycol-6000 by molecular dynamics method showed that the highest release rate of desloratadine was achieved at 1:1 (5.47±1.11 %), 1:2 (5.39±0.51 %) ratios and the lowest at 1:5 (3.03 ± 0.00 %). The obtained results indicate the promising use of solid dispersions "desloratadine – polyethylene glycol-6000" (1:1 ratio).
Keywords: Modeling, release, Desloratadine, Polyethylene glycol-6000, Molecular dynamics
Funding: The research was funded by the Russian Science Foundation grant No. 24-25-20015, https://rscf.ru/project/24-25-20015/.
For citation: Polkovnikova Yu. A., Tulskaya U., Semenov V. N, Slivkin A. I. Modeling of Desloratadine release process from alloys with Polyethylene glycol-6000 by Molecular dynamics method. *Condensed Matter and Interphases*. 2025;27(2): 260–266. https://doi.org/10.17308/kcmf.2025.27/12803

Research article
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Phase diagram of the system Na_2SO_4 – $In_2(SO_4)_3$. Comparative analysis of Na_2SO_4 – $R_2(SO_4)_3$ systems (R = Al, Ga, Fe, In, Sc, Yb)
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Abstract
Purpose: The phase diagram of the system of sodium sulfate with indium sulfate has been studied for the first time.
Experimental: Thermal and X-ray phase analysis (XRD) techniques, including high-temperature analysis, were used.
Conclusions: In the Na_2SO_4 - $In_2(SO_4)_3$ system determined a several substances. The $NaInSO_4$ compound incongruently melted at 800 °C. The $Na_3In(SO_4)_3$ compound has polymorphic transformations at 210 and 580 °C, and decomposes in the solid state at 680 °C. The compound containing 7±1 mol. % $In_2(SO_4)_3$ (ϕ phase), changing to the solid solution at 540 °C. The eutectic coordinates are 710 °C, 18 mol. % $In_2(SO_4)_3$. The solid solution region based on α-Na_2SO_4 is 11±1 mol. % $In_2(SO_4)_3$. The solid solution melting curves show a maximum at 895 °C and 3 mol. % $In_2(SO_4)_3$. According to XRD data, the $NaInSO_4$ compound crystallizes in the structural type of javapaite - $KFe(SO_4)_2$ (monoclinic space group (*C*2/m) with lattice parameters *a* = 8.024 Å, *b* = 5.069 Å, *c* = 7.211 Å, β = 90.6°), and is isostructural to compounds of similar composition with aluminum, gallium, iron, chromium, vanadium and rhodium sulfates. Low-temperature modification $Na_3In(SO_4)_3$ crystallizes in trigonal space group (*R*-3) with lattice parameters *a* = 13.970 Å, *c* = 8.871 Å), and is isostructurally similar to similar compounds with sulfates of aluminum, gallium, iron (III), vanadium, rhodium, scandium. X-ray diffraction pattern of the mid-temperature modification $Na_3In(SO_4)_3$ is indexed in monoclinic space group (*P*21/c) with lattice parameters *a* = 16.187(4) Å, *b* = 13.584(3) Å, *c* = 9.639(2) Å, β = 91.6°. The X-ray diagram of the ϕ phase is indexed in monoclinic space group (*P*21/c) with lattice parameters *a* = 7.836 Å, *b* = 14.845 Å, *c* = 4.57 Å, β = 91.14°.

Keywords: Sodium sulfate, Indium sulfate, Aluminum sulfate, Gallium sulfate, Iron sulfate, Scandium sulfate, Ytterbium sulfate, Phase diagrams, Solid solutions, Isomorphism
For citation: Proydakova V. Yu., Voronov V. V., Kuznetsov S. V., Nekrylov I. N., Zavrazhnov A. Yu., Fedorov P. P. Phase diagram of the Na_2SO_4 – $In_2(SO_4)_3$ system. Comparative analysis of the Na_2SO_4 – $R_2(SO_4)_3$ (R = Al, Ga, Fe, In, Sc, Yb). *Condensed Matter and Interphases*. 2025;27(2): 267–277. https://doi.org/10.17308/kcmf.2025.27/12805

Research article
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Investigation of the transformation of the surface architecture of zinc oxide powders synthesized by grinding during etching with argon ions

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Abstract
Purpose: The aim of the work is to study by X-ray photoelectron spectroscopy the transformation of the surface architecture of zinc oxide powders, previously obtained by mechanical milling, during their etching with argon ions.
Experimental: The etching was carried out in two steps of 30 s duration each at a current of 1 μA. It was found that on the surface of initial powders 45 % of zinc is a part of the crystal lattice of ZnO, and the remaining 55 % exist in the form of hydroxide.
Conclusions: The first etching step reduced the fraction of hydroxyl groups on the surface to 1 per 5 zinc cations in the ZnO lattice, and further etching showed the impossibility of deeper purification of the sample from OH-groups. In contrast, the carbon atoms almost completely left the powder surface after the end of the second etching step.

Keywords: Zinc oxide, Etching, X-ray photoelectron spectroscopy, Surface
Funding: The research was supported by the Russian Science Foundation grant No. 23-29-00844, https://rscf.ru/project/23-29-00844/.
Acknowledgements: The measurements were partially conducted using the equipment of the Research Park of St. Petersburg State University "Centre for Physical methods of surface investigation".
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Research article
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Analysis of anisotropic heat and thermal diffusivity of thermally expanded graphite

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Abstract
Purpose: This paper aims to look into the anisotropic thermal diffusivity of thermally expanded graphite (TEG) foil using flash method. Its structure is compared with graphene oxide (GO) multilayer foil. Morphology, diffractogram and surface profilometry of TEG and GO produced by two different manufacturing processes are demonstrated. TEG was made of intercalated graphite by thermolysis, and GO was made by microwave-assisted graphite oxide peeling (MEGO).
Experimental: The paper studies temperature distribution in the TEG sample as a result of continuous exposure to laser radiation and compares it to those of copper and aluminum samples.
Conclusions: It also provides a perspective on possible application of TEG in heat transfer.

Keywords: Two-dimensional allotropic modification of carbon, Graphene, Thermally expanded graphite, Anisotropy, Cooling
For citation: Prokhorov D. A., Rybin M. G., Zuev S. M. Analysis of anisotropic heat and thermal diffusivity of thermally expanded graphite. *Condensed Matter and Interphases*. 2025;27(2): 284–292. https://doi.org/10.17308/kcmf.2025.27/12809

Research article
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Structures for photocatalysis based on ZnO with Ag nanoparticles

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Abstract
Purpose: This paper aims to establish the regularities of the deposited silver influence on the catalytic activity of zinc oxide. Silver nanoparticles make a promising component for improving the catalytic performance of semiconductor materials through the effect of plasmonics.
Experimental: The experimental part included synthesis of specimens with different silver content from 0.2 to 2 wt %. SEM images and AFM scans of the powders were obtained to characterize the specimen surface. EDX spectra and elemental mapping were obtained to

analyze the composition. As a result, the uniform deposition of silver on the surface of zinc oxide and the agreement of the estimated composition with the obtained were confirmed. Catalyst activity was evaluated by the degree of degradation of the organic dye Rhodamine 6G. The effect of deposited silver on ZnO surface was analyzed.
Conclusions: The deposition of 0.2 wt % silver increases the activity by 58 %, while addition of 2 wt % leads to an increase in activity by 92 %. According to the data obtained, a positive effect of deposited silver on the photocatalytic activity of zinc oxide was found. Dependence of activity change on the amount of silver reaches saturation when 2 wt % of silver is reached.
Keywords: Zinc oxide, Silver nanoparticles, Photocatalysis, Heterojunction, Ecology
For citation: Radaykin D. G., Moshnikov V. A. Structures for photocatalysis based on ZnO with Ag nanoparticles. *Condensed Matter and Interphases*. 2025;27(2): 293–301. https://doi.org/10.17308/kcmf.2025.27/12806

Research article
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Structural and optical properties of Mg-doped ZnO films obtained by spray pyrolysis
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Abstract
Purpose: The paper aims to determine the optimal technological conditions for preparing metal oxide films by spray pyrolysis, as well as to study their structural and optical parameters. Zinc oxide thin films have an important combination of properties for practical application including transparency in the visible range of electromagnetic radiation and low electrical resistance which is provided by a large value of the bandgap width and by obtaining non-stoichiometric compositions or by introducing appropriate alloying elements. The possibility of practical application of ZnO thin films also depends on their optical and electrical properties.
Methods: Thin films of unalloyed zinc oxide as well as ZnO films doped with magnesium with different percentages from 1 to 15 at. % were prepared by spray pyrolysis. Structural and optical properties of magnesium-doped zinc oxide thin films were studied. Through X-ray diffraction analysis it was found that all films are polycrystalline with hexagonal wurtzite structure and crystallographic orientation (002) aligned or oriented along the plane of the substrate.
Conclusions: Studies of optical properties by UV-visible spectrophotometry showed that transmittance of magnesium-doped zinc oxide thin films increased from 70 to about 85 %, and the bandgap width increased from 3.20 to 3.42 eV. These properties of magnesium-doped ZnO thin films demonstrate their high potential for efficient use in many optoelectronic devices and instruments such as solar cells, gas sensors, allow their use as photocatalysts, etc.
Keywords: ZnO thin films, Mg doping, Spray pyrolysis method, Structural properties, Optical properties
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Research article
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Diffractometric studies of the PA MBE grown of GaN layers on silicon substrates without their nitridation and an intermediate AlN nucleation layers
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Abstract
Purpose: The paper describes structural features of the growth of GaN layers synthesized by plasma-assisted molecular beam epitaxy on silicon substrates without substrate nitridation and without the formation of an aluminum-containing interlayer.
Experimental: High-resolution X-ray diffractometry was used to show that the proposed method can be used to grow strain-free GaN films. It was found that in GaN layers grown directly on the Si substrate after its surface passivation by Ga atoms, the value of residual strain was at 300 MPa, while the use of indium atoms as a surfactant during the growth of the GaN layer resulted in a higher residual strain.
Conclusions: The obtained results are important for understanding the viability of the proposed approach for the formation of GaN layers directly integrated with Si without substrate nitridation and the formation of an aluminum-containing buffer. This method opens new opportunities for designing AIIIN-based optoelectronic devices.
Keywords: Plasma-assisted molecular beam epitaxy, GaN layers, Silicon substrate, X-ray diffraction, Strain-free GaN films
Funding: The study was carried out within the framework of the grant of the Ministry of Education and Science of the Russian Federation (project No. FZGU-2023-0006). PA MBE synthesis of the samples was carried out as a part of the grant provided by the Ministry of Science and Higher Education of the Russian Federation (grant No. FSRM-2023-0006).
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Research article
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Effect of the re-emitting layer of organic thin film on the efficiency of silicon solar cells
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Abstract
Purpose: Photovoltaic solar energy conversion technologies represent promising pathways to clean and renewable energy production. Research on organic solar cells is actively developing, especially in the last decade it has attracted scientific and economic interest driven by the rapid increase in energy conversion efficiency. In recent years, luminescent materials capable of converting a broad spectrum of light into photons of a specific wavelength have been synthesized and used to minimize losses in the solar cell-based energy conversion process. This paper presents a study of the optical and luminescent properties of thin films of copper complexes $C_{62}H_{50}Cu_2I_2N_8P_2$.
Experimental: It is proposed to use this material as a re-emitting layer on the surface of a solar cell in order to increase the coefficient of performance (COP) of the latter by converting energy from the ultraviolet range to the visible range. A study of the volt-ampere characteristics of a pure single-crystal solar cell and a cell with an re-emitting copper complex layer has been carried out.
Conclusions: It is shown that deposition of $C_{62}H_{50}Cu_2I_2N_8P_2$ on the surface of solar cells allows increasing the efficiency of converters by 1.45 % in the ultraviolet range at low economic costs. Mechanisms for enhancing energy conversion are discussed and recent experimental results on similar studies are analyzed.
Keywords: Solar cell, Photovoltaic converters, Optical spectrum, Luminescence, Thin films, Copper complexes
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Short communication

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Complexation processes in aqueous solutions of lead acetate and thiourea
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Abstract
Purpose: The aim of the article is to study the processes of comp lexation in aqueous solutions containing lead acetate and thiourea and to establish the optimal concentration regions for the existence of thiocarbamide coordination compounds.
Modeling: The study of ionic equilibria was carried out by means of theoretical calculation taking into account the stability constants of various complex forms. Slices of concentration dependences of fractions of coordination compounds on initial concentrations of lead ions and thiourea, as well as predominance diagrams and distribution diagrams in three-dimensional space were constructed using the COMSOL Multiphysics application package by the Newton-Raphson method.
Conclusions: concentration ranges of existence of coordination compounds formed in aqueous solutions of lead acetate and thiourea at varying concentrations of components have been determined. It was revealed that at low concentrations of lead salt in solution the homogeneously liganded thiourea complexes dominate. With increasing thiocarbamide concentration, the total fraction of homogeneously liganded and dissimilarly liganded thiourea coordination compounds increases.
Keywords: Thiourea coordination compounds, Complexation, Distribution diagrams, Predominance diagram, Lead sulfide films, Aerosol pyrolysis method
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