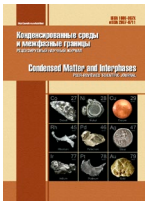

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Аннотации на английском языке

Special issue of the journal "Condensed Matter and Interphases": "Physicochemical Analysis in Materials Science" (continued)

Review

Review article
https://doi.org/10.17308/kcmf.2025.27/12483

Features of synthesis and properties of new materials based on monoisotopic silicon and germanium. Review

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Abstract
This paper reviews scientific works on the preparation and properties of isotopically enriched silicon and germanium, along with their compounds. It covers the technological aspects and peculiarities of synthetic methods with the deep purification processes for obtaining isotopically enriched silicon and germanium compounds. The review also discusses the production of polycrystalline and single-crystal samples with varying degrees of isotopic and chemical purity. The results of a study investigating the physicochemical characteristics of both simple and complex substances derived from isotopically enriched silicon and germanium are presented. These studies indicate that the isotopic composition of silicon and germanium significantly affects heat capacity, thermal conductivity, and light absorption processes. Finally, the paper explores current applications of substances and materials based on isotopically enriched silicon and germanium.

Keywords: Silicon, Germanium, Isotopes, Hydrides, Materials
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Review article
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Advanced methods for preparing especially pure glasses based on germanium and gallium chalcogenides. Part 1. Synthesis via volatile and low-melting compounds. Review

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Abstract
Glasses based on germanium and gallium chalcogenides are promising optical materials for the near and mid-infrared (IR) regions. They are used to develop fiber-optic sensors, sources of supercontinuum, luminescent and laser radiation, glass-ceramic materials with improved mechanical properties, memory cells, and other optical and optoelectronic devices. The most important characteristic of chalcogenide glasses is the content of limiting impurities that have the most negative effect on their optical properties. Conventional methods for producing these materials include melting simple substances with getters in evacuated silica-glass ampoules and then distilling the melt. These methods do not allow achieving extremely low concentrations of impurities that do not affect optical transparency of glasses. Therefore, new approaches need to be developed.
The purpose of the review is to systematize the scientific information related to the methods for preparing especially pure chalcogenide glasses which have been developed over the past 15 years at the Institute of Chemistry of High Purity Substances of the Russian Academy of Sciences. The methods discussed in the first part of the paper include: 1) synthesis of *p*-element chalcogenides via volatile iodides; 2) preparing a batch by thermal decomposition of germanium sulfide and selenide iodides; 3) synthesis and deep purification of germanium monochalcogenides. The developed methods made it possible to reduce the content of hydrogen, oxygen, and carbon impurities and heterogeneous inclusions in chalcogenide glasses by 1–2 orders of magnitude as compared to conventional methods. In conclusion, the article discusses the possibilities for further reduction of the content of impurities in glasses based on germanium and gallium chalcogenides to achieve extremely low optical losses.

Keywords: Chalcogenide glasses, Especially pure substances, Optical materials, Synthesis, IR spectrometry, Chemical transport reactions
Funding: The research was carried out with the financial support of the national project "Science and Universities" at the laboratory "Ultra-pure chalcogenide glasses for mid-infrared photonics", state order FFSR-2024-0001 and the Research and Education Centre of the Nizhny Novgorod Region within the framework of the "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 1. Synthesis via volatile and low-melting compounds. Review. *Condensed Matter and Interphases*. 2025;27(1): 16–28. https://doi.org/10.17308/kcmf.2025.27/12482

Аннотации на английском языке

Review article
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Phases with layered (AB) and "defective" (A_2B_3) structures in A^{III}–B^{VI} systems. Part 2. Phase diagrams and approaches to some problems of reproducible synthesis in A^{III}– B^{VI} systems. Review
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Abstract
The paper analyzes phase diagrams of A^{III}–B^{VI} systems and phase equilibria involving crystalline compounds formed in these systems. The location of each solid binary phase mainly related to mono- and sesquisulfides families and selenides of aluminum, gallium, and indium on *T-x*-diagrams is discussed in detail. The homogeneity regions of these phases were also analyzed if the necessary data were available. For polymorphic (or close to them) transformations, the nature of the occurring structural transformations was described and the temperature stability of various modifications of similar composition was analyzed. Using examples of several systems, it was shown how, by changing the experimental conditions, it is possible to reproducibly obtain compounds with the required structure (even for different polytypes of structures with very similar structures of individual layers) and the required composition (including those within the regions of phase homogeneity). Various methods of reproducible inorganic synthesis were considered, taking into account the features of the phase diagram and phase equilibria. In conclusion, current and partially still unresolved issues concerning the characteristics of the $A_2^{III}B_3^{VI}$ and $A_1^{III}B_1^{VI}$ compounds were analyzed.
Keywords: Chalcogenides, *A*(III)*B*(VI), Stoichiometric vacancies, Phase diagrams, Phase equilibria
For citation: Zavrazhnov A. Y., Brezhnev N. Y., Nekrylov I. N., Kosyakov A. V. Phases with layered (AB) and "defective" (A_2B_3) structures in A^{III}- B^{VI} systems. Part 2. Phase diagrams and approaches to some problems of reproducible synthesis in A^{III}– B^{VI} systems. Review. *Condensed Matter and Interphases*. 2025;26(1): 29–47. https://doi.org/10.17308/kcmf.2025.27/12484

Original articles

Research article
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Thermodynamic study of zinc antimonides by the electromotive force measurements
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Abstract
Zinc antimonides and phases based on them are of great interest as earth-abundant, low-cost, and environmentally friendly thermoelectric materials. The present work demonstrates the results of a thermodynamic study of the ZnSb and Zn_4Sb_3 compounds by a low-temperature electromotive force (emf) method with a glycerol electrolyte in the 300-430 K temperatures range.
Measurements were performed using equilibrium samples from the ZnSb+Sb and ZnSb+Zn_4Sb_3 two-phase regions of the Zn-Sb binary system. The phase compositions of prepared samples were controlled by means of the powder X-ray diffraction (PXRD) method. Using the least square method, the linear equations of temperature dependences of the emf data were obtained.
Based on these equations and relevant thermodynamic expressions, the partial molar Gibbs free energy, enthalpy, and entropy of zinc in alloys were calculated. Utilizing the phase diagram of the Zn-Sb system, the virtual-cell reactions for both binary compounds were determined, based on which their standard thermodynamic functions of formation and standard entropies were calculated. A comparative analysis of the obtained results with available literature data was carried out.
The results of the current work are highly accurate and can be considered a new contribution to the thermodynamics of zinc antimonides.
Keywords: ZnSb, Zn_4Sb_3, *emf* method, Electrochemical cells, Glycerol electrolyte, Thermodynamic functions
For citation: Aghayeva A. R., Mammadova S. H., Babanly D. M., Jafarov Ya. I., Tagiyev D. B. Thermodynamic study of zinc antimonides by the electromotive force measurements. *Condensed Matter and Interphases*. 2025;27(1): 48–56. https://doi.org/10.17308/kcmf.2025.27/12485

Research article
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Refinement of the phase diagram of the MnSe–In_2Se_3 system and the crystal structures of $MnIn_2Se_4$ and $Mn_2In_2Se_5$ compounds
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Abstract
Complex chalcogenides based on transition elements, in particular ternary compounds of the AB_2X_4 type (M = Mn, Fe, Co, Ni; B = Ga, In, Sb, Bi; X = S, Se, Te) are among the important functional materials. Compounds of this class exhibit the phenomena of electronically or

optically controlled magnetism and are very promising for the creation of lasers, light modulators, photodetectors, and other functional devices controlled by a magnetic field. Recent studies demonstrated that these compounds can also find application in photocatalysis, photovoltaics, and thermoelectric converters.

The study presents new data on phase equilibria in the MnSe–In_2Se_3 system, obtained by differential thermal analysis, X-ray phase analysis, and scanning electron microscopy. Two ternary compounds, $MnIn_2Se_4$ with congruent melting at 1193 K and $Mn_2In_2Se_5$, melting incongruently at 1196 K, were formed in the system. The first is a phase of variable composition and has a 5–6 mol. % homogeneity region towards an excess of In_2Se_3. Based on powder diffraction data, the Rietveld method was used to refine the crystal structures and lattice parameters of both ternary compounds.

Keywords: Manganese-indium selenides, Phase equilibria, Homogeneity region, Crystal structure, Rietveld method

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Research article

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A universal algorithm for the calculation of vapor-liquid equilibrium diagrams in quasi-simple multicomponent systems

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Abstract

The purpose of the study was to consider isothermal vapor-liquid diagrams of quasi-simple systems and to develop a universal algorithm for the calculation of isothermal vapor-liquid diagrams of these systems independent of the type of valence of the electrolyte, the number of components in the system, and the types of solid solutions. The suggested analogues of the three Gibbs–Konovalov and Gibbs–Roozeboom laws are true when moving along the univariant equilibrium lines on the solubility diagrams of systems with a random number of components.

The study did not involve any experiments. The suggested algorithm was applied for the description of solubility (solid-liquid) diagrams and vapor-liquid equilibrium diagrams of three- and four-component systems with one, two, or three volatile components. In all the cases, the results of thermodynamic first-principles calculations agreed well with the experimental data presented in the literature.

Both the experimental data presented in the literature and the results of the thermodynamic first-principles calculation performed by the authors are also in good agreement with the suggested analogues of the Gibbs–Konovalov and Gibbs–Roozeboom laws.

Keywords: Zdanovskii's rule, Quasi-simple systems, Vapor-liquid equilibrium diagrams, Partial molar Gibbs energy, Analogues, Gibbs–Konovalov's laws, Gibbs–Roozeboom rules

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Articles of issue 1
Original articles

Research article

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Analysis of the crystalline quality of bulk $In_{0.83}Ga(Al)_{0.17}$ layers formed on metamorphic InAlAs/InP buffer layers with linear and nonlinearcomposition gradients

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Abstract

This paper investigates the effectiveness of metamorphic InAlAs buffer layers with linear and root-like dependence of the In mole fraction in the composition for the growth of bulk $In_{0.83}Ga(Al)_{0.17}As$ layers on InP substrates. The analysis of the X-ray diffraction reciprocal space maps showed that in both cases $In_{0.83}Ga(Al)_{0.17}As$ layers were partially strain-free. One of the mechanisms of strain relaxation during the

growth of the linearly graded buffer layer is the rotation of the crystal lattice, while the mechanism of strain relaxation during the growth of the convex-graded buffer layer is a 0.82° tilt of the crystal lattice without any rotation. According to the images obtained by transmission electron microscopy, the density of threading dislocations in the upper InGaAs layers grown on the buffer layer with a linear composition gradient is ~ $5 \cdot 10^8$ cm^{-2}.

Keywords: Metamorphic buffer layers, Reciprocal space mapping of X-ray diffraction intensity, Transmission electron microscopy, Molecular beam epitaxy

Funding: The study was funded by the Russian Science Foundation, research project No. 22-79-00146.

For citation: Vasilkova E. I., Pirogov E. V., Nevedomsky V. N., Barantsev O. V., Voropaev K. O., Vasiliev A. A., Karachinsky L. Ya., Novikov I. I., Sobolev M. S. Analysis of the crystalline quality of bulk $In_{0.83}Ga(Al)_{0.17}As$ layers formed on metamorphic InAlAs/InP buffer layers with linear and nonlinearcomposition gradients. *Condensed Matter and Interphases*. 2025;27(1): 86–95. https://doi.org/10.17308/kcmf.2025.27/12624

Research article

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Study of hyperfine interactions in spinel cobalt ferrite $CoFe_2O_4$ doped with Hf, Lu, and Yb using Mössbauer spectroscopy and perturbed γ-γ angular correlation

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Abstract

We studied hyperfine interactions (HFI) in spinel cobalt ferrite (ferrospinel) $CoFe_2O_4$ doped with Lu, Yb, and Hf (1 wt. %) by Mössbauer spectroscopy (MS) on ^{57}Fe nuclei. The interactions indicate the presence ($CoFe_2O_4$:Lu – 11 %, $CoFe_2O_4$:Yb – 23.4%) and the absence ($CoFe_2O_4$:Hf) of additional phases. The study revealed a significant change in the HFI parameters on ^{57}Fe nuclei in the octahedral sites in ferrospinels doped with Hf, Lu, and Yb. However, the relative influence of the impurity on ^{57}Fe nuclei in the tetrahedral sites was insignificant. The parameters of hyperfine fields on ^{172}Yb nuclei in cobalt ferrite were obtained by the method of perturbed γ-γ angular correlations (PAC). The ^{172}Yb ions were introduced into the sample using two methods: by adding ^{172}Hf and ^{172}Lu isotopes. A significant difference in the HFI parameters for these two cases was revealed. The local environment of ^{172}Yb ions appears to be different in the two variants of isotope introduction into the sample (Hf or Lu). The difference in the HFI parameters persisted in the temperature range of 300 - 1000 K.

It was determined that the different effects of Hf and Lu on the parameters (electric field gradient, magnetic field, and isomer shift) of the HFI in the sample are revealed by both MS and PAC methods, irrespective of the amount of the dopant. According to the MS data, Hf and Lu do not lead to significant changes in the HFI parameters in the tetrahedral sites ("Sextet 1"), but have a significantly different effect on the same parameters in the octahedral sites ("Sextet 2"). A similar pattern was observed using the PAC method: replacing Hf with Lu did not reveal any changes in the HFI parameters in one of the sites (the octahedral site), but indicated a significant change in the other site.

Keywords: Mössbauer spectroscopy, Perturbed correlations, Spinels, Oxides, Ferrites

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Research article

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Chemical vapor deposition of $Tm_3Fe_5O_{12}$ epitaxial films, investigation of their structure and properties in the terahertz range

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Abstract

In this study, for the search and development of new spintronic materials, thin films of $Tm_3Fe_5O_{12}$ iron garnet were obtained by the metalorganic chemical vapor deposition (MOCVD) on single-crystal $Gd_3Ga_5O_{12}$(111) – GGG and $Y_3Al_5O_{12}$(111) – YAG substrates. The $Tm_3Fe_5O_{12}$ films were investigated using X-ray diffraction, Energy dispersive X-Ray microanalysis, Raman spectroscopy and terahertz (THz) pulsed spectroscopy.

The epitaxial nature of films deposited on substrates of both types demonstrated. It was found that the growth of garnet film under the high-temperature vacuum conditions of MOCVD on a GGG substrate is complicated by the evaporation of gallium oxide, which causes the introduction of iron oxide into the surface layer of the substrate, enrichment of the adjacent layer of the film with thulium oxide and the formation of non-stoichiometric garnet with antisite defects.

It was concluded that YAG substrates are more promising, since the heteroepitaxy of iron garnets on them does not have such complications.

Keywords: Thin films, Iron garnets, MOCVD, Structure, Antisite defects, Raman spectroscopy, Terahertz spectroscopy

Funding: Work on MOCVD film production was carried out using equipment purchased using funds from the Moscow University Development Program. The study was carried out with the financial support of the Interdisciplinary Scientific and Educational Schools of Moscow University (Project No. 24-Ш06-13).

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Research article

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Topography and microrelief electroless Ni-P coatings at different loading densities

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Abstract

The aim of this study was to investigate the growth processes of Ni-P coatings at different loading densities of the electroless nickel plating bath. The Ni-P coatings can be used to improve the thermal and corrosion resistance of optical fiber used to manufacture sensors of various physical quantities.

When depositing coatings on optical fiber, the loading density is an important parameter. The study investigated the influence of loading density on the topography, microrelief, roughness, and growth mechanism of Ni-P coatings using non-contact high-resolution optical profilometry. An increase in loading density from 0.5 to 3.0 dm^2/l did not lead to a significant change in the roughness parameters of the coatings. During the growth of coatings, "spheroids" strongly elongated in the plane of the substrate were formed on the surface. An analysis of growth processes was carried out within the framework of the layered growth mechanism. The growth rates of spheroids in normal and lateral directions were assessed. An increase in the loading density led to a decrease in the growth of spheroids in the normal direction, while the growth rate in the lateral direction was maximal at a loading density of 2 dm^2/l. Statistical analysis of the sizes of the "spheroids" showed that their distribution deviated from the normal law, which may be due to the fact that not only individual spheroids, but also their aggregates were considered in calculations. Another reason for the deviation may be a decrease in the proportion of the active surface on which the coating is deposited as the loading density increases.

Since increasing the loading density from 0.5 to 3.0 dm^2/l did not lead to a significant change in the roughness parameters even with coating thickness of ~ 8 μm or higher; deposition of coatings with the thickness up to 3.5 μm thick on optical fibers can be carried out at the specified loading densities with acceptable surface roughness.

Keywords: Optical fiber, Ni-P coatings, Electroless deposition, Non-contact profilometry, Topography, Microrelief, Roughness, Growth mechanism, "Spheroids", Statistical analysis

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Research article

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Coulometric analysis method for determining the concentration and degree of oxidation of vanadium in the electrolyte of a vanadium flow battery using a hydrogen vanadium cell

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Abstract

Determining the vanadium content and the average degree of oxidation of vanadium ions in an electrolyte is a highly important task, both in the production and operation of vanadium flow batteries and in scientific research aimed at improving the performance characteristics of electrolytes throughout their entire life cycle. This article proposes a solution to this issue using the coulometric analysis of electrolyte samples circulating through a cell with a membrane-electrode unit consisting of a gas diffusion hydrogen electrode, a proton exchange membrane, and a liquid flow electrode. The coulometric analysis involves the oxidation of the sample to the highest degree of vanadium oxidation with further reduction to an oxidation state of +4. The parameters of the procedure (polarization modes and completion conditions) were chosen in order to minimize the relative error in determining the concentration of vanadium up to 5% and the average degree of oxidation up to 2% based on model composition electrolytes with different concentrations and degrees of vanadium oxidation, including sulfuric acid, as well as mixed acid (H_2SO_4 + HCl) compositions.

Keywords: Vanadium electrolyte, Vanadium flow batteries, Coulometry, Hydrogen electrode, Concentration, Degree of oxidation of vanadium

Funding: The study was supported by the Russian Science Foundation, project No. 22-73-00157.

For citation: Petukhova E. A., Ershova V. S. Terentyev A. V., Ruban E. A., Pichugov R. D., Konev D. V., Usenko A. A. Coulometric analysis method for determining the concentration and degree of oxidation of vanadium in the electrolyte of a vanadium flow battery using a hydrogen vanadium cell. *Condensed Matter and Interphases*. 2025;27(1): 128–138. https://doi.org/10.17308/kcmf.2025.27/12490

Research article
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The role of nanofillers of various nature in the morphological changes of the polymer binder for plywood production

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Abstract
Nanomodification of the adhesive composition is one of the promising methods for improving the quality of wood laminated materials. Morphological changes in nanostructures make it possible to control the functional characteristics of the resulting nanocomposites. The shape and distribution of nanomodifiers of nanocellulose and multi-walled carbon nanotubes of urea-formaldehyde resin used to produce plywood have been studied by atomic force microscopy. The phase composition and crystal structure of biological and carbon nanofillers of the binder are investigated. Data on the qualitative and quantitative composition, structural state of nanocrystalline cellulose and multi-walled carbon nanotubes, as well as cured resin in pure and modified form, were obtained by X-ray diffractometry. The microrelief of the surface of the cured binder in the presence of multi–walled carbon nanotubes is characterized by uniformly distributed nanoclusions of 50 nm – 1 μm; and nanoclusions of 70 nm - 2 μm in the case of resin modification with nanocrystalline cellulose. Unmodified urea-formaldehyde resin is characterized by a low degree of crystallinity: the crystallite size is 10 nm. When modifying the resin with multi–walled carbon nanotubes, the crystal size increases to 18 nm, and when modified with nanocrystalline cellulose - up to 15 nm. The most probable type of lattice of the resin under study is a primitive cubic one with a parameter a = 0.840 nm. An increase in the volume of the unit cell of resin modified with multi-walled carbon nanotubes (a = 0.844 nm) and nanocrystalline cellulose (a = 0.842 nm) is observed. An increase in the size of the crystalline regions in the resin, as well as an increase in the volume of the resin unit cell as a result of the use of nanomodifiers, can help improve the performance of plywood.

Keywords: Crystal lattice, Urea-formaldehyde resin, Multi-walled carbon nanotubes, Nanocrystalline cellulose, Modification
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Theoretical and experimental study of the niobium dioxide electronic structure

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Abstract
The investigation of the niobium dioxide electron-energy structure is presented in the paper. The electronic structure computer modeling of the NbO_2 with a rutile crystal structure has been performed using linearized augmented plane wave method. The energy band structure as well as total and partial densities of electronic states are calculated.
Experimental studies of the NbO_2 sample electronic structure were carried out using synchrotron and laboratory X-rays sources. The X-ray photoelectron spectrum of the valence band and subvalent states of NbO_2 and the spectrum of the X-ray absorption near edge structure near K-edge of the oxygen atom in NbO_2 have been recorded.
The spectra of the X-ray absorption near edge structure of the oxygen and niobium atoms K-edges are modeled. The calculated spectra make it possible to reliably interpret the data from the synchrotron experiment. It is shown that for NbO_2 the spectrum calculated for the ground energy state without using the supercell and core hole modeling method demonstrates high agreement with the experiment.

Keywords: Computer modeling, Niobium dioxide, Electronic structure, Density of states, XANES, XPS, Core hole, Rutile
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Monte Carlo simulation of interfacial adhesion between geopolymer binders and mineral aggregates

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Abstract
Silico-aluminophosphate and alkali-aluminosilicate geopolymers are increasingly popular as a green alternative to traditional Portland cement concrete used in the construction industry. In geopolymer concretes and mortars, the aggregate-matrix interface plays a major role in the fracture mechanisms. The adhesion strength between the mineral aggregate and the geopolymer matrix is mainly determined by the chemical nature of the components of the aggregate-geopolymer interface. However, this aspect remains insufficiently studied. Therefore, we used a Monte Carlo simulation to investigate adhesive behavior and interfacial interaction mechanisms of a cyclic aluminosilicate oligomer forming the structure of a geopolymer gel with mineral aggregates.

Аннотации на английском языке

The study determined the low-energy equilibrium configurations of the structure of oligomers adsorbed on the surface of quartz, calcite, albite, and microcline, as well as the adsorption energies.
Keywords: Geopolymer, Interfacial adhesion, Mineral aggregate, Quartz, Calcite, Albite, Microcline, Monte Carlo method
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