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Аннотации на английском языке

Research article

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Synthesis and study of the properties of synthetic analogues of the mineral naffildite with the participation of rare earth elements

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Abstract

In recent years, there has been a significant increase in interest in ternary and quaternary compounds with the participation of rare earth elements (REE), as well as copper, antimony, and bismuth, which have a wider range of physical properties. Due to their valuable physical properties, they have become promising targets of research for modern materials science. Therefore, the purpose of this work is to study the properties of synthetic analogues of naffildite with the participation of rare earth elements.

The samples were synthesised from ternary sulphides (in the case of obtaining $\text{Cu}_2\text{LaSb}_3\text{S}_7$, $\text{Cu}_2\text{CeSb}_3\text{S}_7$, $\text{Cu}_2\text{PrSb}_3\text{S}_7$ and $\text{Cu}_2\text{NdSb}_3\text{S}_7$) by fusion in sealed quartz ampoules, preliminarily evacuated to a residual pressure of 10^{-3} mmHg at 950–1100 K for 8 hours. The remaining antimony and bismuth-containing analogues, due to the peritectic nature of formation, were synthesised through batches ($2\text{Cu} + \text{Ln} + 3\text{Sb}(\text{Bi}) + 7\text{S}$) from especially pure elements. After completion of the reaction, homogenizing annealing was carried out for a month at 600–700 K, depending on the composition. The obtained samples were investigated by differential thermal (DTA), X-ray phase (XRD) and microstructural (MSA) analyzes, as well as by measuring the microhardness and determining the density.

Compounds of the $\text{Cu}_2\text{LnSb}_3\text{S}_7$ or $\text{Cu}_2\text{LnBi}_3\text{S}_7$ (Ln – REE) type have been synthesised by direct synthesis from elements or from the ligature $\text{CuSb}_2(\text{CuBi}_2\text{S}_2)$ and $\text{LnSb}_2(\text{LnBi}_2\text{S}_2)$. It was found that they are isostructural and crystallize in the orthorhombic system ($\text{Cu}_2\text{LnSb}_3\text{S}_7$, $a = 14.490 \div 14.264$, $b = 21.422 \div 21.206$, $c = 3.902 - 3.804$ Å; $\text{Cu}_2\text{LnBi}_3\text{S}_7$, $a = 14.722 \div 14.506$, $b = 21.864 \div 21.564$, $c = 4.142 \div 3.464$ Å; $Z = 4$, simple group Pbnm or Pbn₂) and belong to the structure type of naffildite $\text{Pb}_2\text{Cu}(\text{Pb}, \text{Bi})\text{Bi}_2\text{S}_7$. $\text{Cu}_2\text{LaSb}_3\text{S}_7$, $\text{Cu}_2\text{PrSb}_3\text{S}_7$ and $\text{Cu}_2\text{NdSb}_3\text{S}_7$ melt congruently at 975, 985, and 1015 K, respectively, and other compounds are formed by a peritectic reaction.

Keywords: compound, crystal structure, naffildite, lattice parameters, electrical conductivity, thermal electromotive force.

Research article

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A refined phase diagram of the GeTe–Bi₂Te₃ system

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Abstract

Updated phase diagram of the GeTe–Bi₂Te₃ system was constructed using differential thermal, X-ray diffraction analysis and scanning electron microscopy (SEM) results of alloys synthesised with specially developed technology. The refined version significantly differs from those reported so far. The presented phase diagram reflects six ternary compounds: $\text{Ge}_4\text{Bi}_2\text{Te}_7$, $\text{Ge}_3\text{Bi}_2\text{Te}_6$, $\text{Ge}_2\text{Bi}_2\text{Te}_5$, GeBi_2Te_4 , GeBi_4Te_7 , and $\text{GeBi}_6\text{Te}_{10}$.

The study determined that the first two compounds are formed as a result of solid-state reactions at temperatures of 750–800 K, and the latter four are formed as a result of peritectic reactions at 863, 854, 848, and 843 K, respectively. Wide homogeneity regions based on the initial binary compounds were also found. These regions reach 10 mol% at room temperature. The coordinates of eutectic point are 83 mol% Bi₂Te₃ and 838 K. It crystallises at 838 K. It was found that all the identified ternary compounds crystallise in a tetradymite-like layered structure. $\text{Ge}_4\text{Bi}_2\text{Te}_7$, $\text{Ge}_3\text{Bi}_2\text{Te}_6$, $\text{Ge}_2\text{Bi}_2\text{Te}_5$, and GeBi_2Te_4 compounds belong to the $n\text{GeTe-Bi}_2\text{Te}_3$ homologous series. Their crystal lattices are formed by the insertion of GeTe bilayers into the quintuple Bi₂Te₃ layers. GeBi_4Te_7 and $\text{GeBi}_6\text{Te}_{10}$ compounds are representatives of the $\text{GeTe-}m\text{Bi}_2\text{Te}_3$ homologous series and have a mixed-layer structure. The parameters of the crystal lattices of the compounds were determined by the Rietveld method based on their powder diffraction data.

Keywords: Germanium-bismuth tellurides, Phase diagram, Layered tetradymite-like structures, Solid solutions

Research article

<https://doi.org/10.17308/kcmf.2022.24/9051>**Preparation and characterisation of cobalt and cobalt-zinc ferrites for magnetorheological materials****Yu. S. Haiduk¹, E. V. Korobko², D. A. Kotsikau¹, I. A. Svitov¹, A. E. Usenka¹, V. V. Pankov¹**¹Belarusian State University, 4 Nezavisimosty pr., Minsk 220030, Belarus²A. V. Luikov Heat and Mass Transfer Institute of NAS of Belarus, 15 P. Brovki ul., Minsk 220072, Belarus**Abstract**

The aim of this study was to study the structure, morphology, magnetic, and magnetorheological properties of cobalt and cobalt-zinc ferrite powders to be used as a functional component of magnetorheological fluids.

Ferrites of cobalt CoFe_2O_4 and cobalt-zinc $\text{Co}_{0.65}\text{Zn}_{0.35}\text{Fe}_2\text{O}_4$ were obtained by combined hydrolysis of inorganic metal salt in aqueous solutions followed by thermal treatment of the precipitates. The ferrites were studied by means of X-ray phase analysis, scanning electron microscopy, IR spectroscopy, and magnetometry.

The synthesised ferrites are polydispersed powders with the size of primary particles of 300–400 nm and the size of the coherent scattering regions of 22–33 nm. They demonstrate a high shear stress in magnetorheological suspensions, which is 2.5 times higher than that of the nanosized particles. High-temperature annealing results in a significant increase in the specific magnetisation of the powders, as well as the shear stress in suspensions prepared on their basis. Doping cobalt ferrite with zinc leads to an increase in the specific magnetisation and rheological characteristics.

The studied materials have a high shear stress in suspensions (~ 2.5 kPa at 650 mT) and can be used as functional fillers for magnetorheological materials.

Keywords: Cobalt ferrite, Cobalt-zinc ferrite, Magnetorheological materials

Research article

<https://doi.org/10.17308/kcmf.2022.24/9052>**Formation of a solvate of manganese(III) acetylacetonate with chloroform****V. P. Zlomanov, R. S. Eshmakov, I. V. Prolubshchikov**

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Abstract

Metal acetylacetonates are coordination compounds consisting of the acetylacetonate anion ($\text{CH}_3\text{COCHCOCH}_3$, indicated as acac) and metal ions. Typically, both oxygen atoms of the anion bind with the metal and form a six-membered chelate ring. The simplest complexes have the formulas $\text{M}(\text{acac})_3$ and $\text{M}(\text{acac})_2$. Many complexes are soluble in organic solvents, and such solutions are used for the synthesis of catalysts. The processes of formation of solvates of acetylacetonates of various metals have not been studied properly. It should be noted that the determination of the composition and properties of solvates is important for understanding the peculiarities of the extraction processes of metal acetylacetonates. Manganese(III) acetylacetonate $\text{Mn}(\text{acac})_3$, for example, is also widely used. The recrystallisation of the complex is most commonly conducted from solutions in chloroform, and in this case, the corresponding solvates may be formed, which can affect the structure and properties of $\text{Mn}(\text{acac})_3$. There are no data on the synthesis conditions and the composition of the solvates of manganese(III) acetylacetonate with chloroform. Therefore, the purpose of this work is to study the possibilities of its formation and to establish the composition of such solvates.

The formation of the solvate in solution was established using Fourier IR spectroscopy by the shift of the absorption band of the C-H chloroform bond. The composition of the $\text{Mn}(\text{acac})_3 \cdot 2\text{CHCl}_3$ solvate was determined using gravimetric analysis.

Keywords: Manganese, Acetylacetonate, Solvate, Gravimetric analysis, IR spectroscopy

Research article

<https://doi.org/10.17308/kcmf.2022.24/9053>**The influence of the physicochemical nature of the components of the $\text{V}_2\text{O}_5/\text{GaAs}$, MnO_2/GaAs , $\text{V}_2\text{O}_5/\text{InP}$, MnO_2/InP , TiO_2/InP , and SnO_2/InP heterostructures and the oxidation conditions on the surface morphology of the synthesised films****A. S. Kovaleva¹, B. V. Sladkopezvtsev¹, A. A. Samsonov¹, S. I. Alferova², D. G. Kovalev¹, S. A. Titov¹, N. D. Pryakhin¹, I. Ya. Mittova¹**¹Voronezh State University, ¹Universitetskaya pl., Voronezh, 394018, Russian Federation²Voronezh State Pedagogical University, 86 ul. Lenina, Voronezh, 394043, Russian Federation**Abstract**

The formation of oxide functional films on the surface of semiconductors is a serious technological challenge, which is even more complicated in the nanometre thickness range. It is necessary to form films with specified values of thickness, resistivity, and a certain surface morphology for practical applications. Such films are used in micro- and optoelectronics, environmental monitoring, and alternative energy devices. The goal of this work is to establish the features of the surface morphology of thin films formed as a result of the thermal oxidation of the MnO_2/GaAs , $\text{V}_2\text{O}_5/\text{GaAs}$, $\text{V}_2\text{O}_5/\text{InP}$, MnO_2/InP , TiO_2/InP , and SnO_2/InP heterostructures depending on the physicochemical nature of the components and the oxidation conditions.

The synthesis of thin films on the InP and GaAs surfaces was carried out by thermal oxidation under the influence of magnetron-deposited layers of chemostimulator-modifiers. The thickness of the formed films and their composition were determined by laser ellipsometry, X-ray phase analysis, and infra-red spectroscopy. The scanning tunnel and atomic force microscopy were used to determine the morphological characteristics of the films and their dependence on the type of semiconductor substrate, the nature of the chemostimulator-modifier, and the conditions of the thermal oxidation.

The application to the GaAs and InP surfaces of the most effective chemostimulator-modifiers (V_2O_5 and MnO_2) of thermal oxidation and higher temperatures of the oxidation process contributed to the formation of smoother and nanostructured films.

Keywords: Gallium arsenide, Indium phosphide, Heterostructure, Thermal oxidation, Surface morphology, Grain size

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Research article

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The interconnection of efficiency and the degree of aggregation of nanofiller in polymer nanocomposites

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Abstract

The rule of mixtures was the first theoretical model, used for a description of the elastic modulus of multicomponent systems, including those of polymer nanocomposites. However, the use of nominal magnitudes of the characteristics of system components in such an approach led to overestimated values of their elastic modulus. Therefore, various modified versions of the rule of mixtures are currently used for this purpose, which significantly complicate its application and do not indicate the physical factors leading to overestimated theoretical results.

In this study, a modified rule of mixtures was proposed, taking into account the decrease in the effective (actual) elastic modulus of the nanofiller in a polymer matrix of the nanocomposite compared to the nominal value determined only by the aggregation of the nanofiller. It is known that the aggregation process is the main negative factor reducing the final properties of nanomaterials, while other factors (for example, the interfacial adhesion level, nanofiller orientation, etc.) depend on the degree of aggregation. The physical sense of the aggregation process is a decrease in the relative proportion of nanofiller-polymer matrix interfacial regions, i.e., the effectiveness of a nanofiller as a reinforcing element of a nanocomposite is determined by its ability to generate high-modulus interfacial regions.

The rule of mixtures modified in this way correctly describes the dependence of the elastic modulus of the nanocomposite on the content of the nanofiller, regardless of the type of the latter (carbon nanotubes, graphene, etc.). Therefore, the nanofiller efficiency indicator can serve as a complex parameter that is characteristic of the nanocomposite quality.

Keywords: The rule of mixtures, Nanocomposite, Carbon nanotubes, Graphene, Aggregation, Elastic modulus, Interfacial regions

Research article

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Characteristics of the formation and composition of $Al_xGa_{1-x}N/AlN/por-Si/Si(111)$ heterostructures grown using a porous silicon buffer layer

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Abstract

In this work, we studied the efficiency of introducing nanoporous silicon as a buffer layer in the growth of $Al_xGa_{1-x}N/AlN/Si(111)$ on a single-crystal silicon by molecular beam growth technology. We also considered its influence on the morphological characteristics and atomic composition of the surface layers of heterostructures. As determined by X-ray diffraction, microscopic, and X-ray photoelectron methods, the heterostructure grown on Si(111) *n*-type monocrystalline silicon wafer with nanoporous por-Si buffer layer has a more homogeneous epitaxial layer, and the surface morphology of the layer is also more homogeneous.

Keywords: Porous silicon buffer layer, Heterostructures, Epitaxy

Research article

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Corrosion inhibition of steel by selected homologues of the class 3-alkyl-5-amino-1H-1,2,4-triazoles in acidic media

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Abstract

The use of hydrochloric acid in the treatment of the bottomhole formation zone leads to the significant corrosion of metals, as well as hydrogen and chloride stress cracking of pump compressor pipes. In order to solve this problem, corrosion inhibitors are added to a hydrochloric acid solution. This article presents the results of a study of the anticorrosive activity of a number of derivatives of the class of 3-alkyl-5-amino-1H-1,2,4-triazole under the conditions of hydrochloric acid corrosion of low-carbon steel.

During the study, selected 3-alkyl-5-amino-1H-1,2,4-triazoles were synthesized. Their structure was confirmed and proved using NMR spectroscopy and HPLC/MS spectrometry. Regularities of the anticorrosive action of the investigated compounds have been established using polarization electrochemical studies and gravimetric direct corrosion tests. Corrosion rates, inhibition coefficients and degrees of protection have been calculated for all inhibitors. The probable mechanism of the inhibitory action of the studied compounds has been substantiated using quantum chemical calculations based on the density functional theory using the Gaussian program.

It was shown that the structure of the alkyl substituents has the greatest effect on the inhibitory activity of the studied compounds. The mechanism was proposed for the adsorption of the inhibitor, which explained the increase in protective properties with an increase in the

length of the alkyl substituent. The high hydrophobicity of the aliphatic fragment, not involved in the chemisorption process, additionally prevents the acid solution from contacting the metal surface, while the heterocyclic moiety ensures the sorption of the inhibitor on the metal surface.

As a result, it was shown that derivatives of the homologous series of 3-alkyl-5-aminotriazole are suitable as inhibitors of acid corrosion of ST-3 steel. The minimum length of a hydrocarbon radical at which significant inhibitory activity was observed is 7 carbon atoms. Protection degrees of 65–85% were achieved when 3-heptyl-5-amino-1H-1,2,4-triazole additives at a concentration of at least 2 g/L were added to the hydrochloric acid solution.

Keywords: Metal corrosion, Steel, corrosion inhibitors, Heterocyclic compounds, Aminotriazoles, Physicochemical research methods, Drilling equipment

Research article

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Specifics of the formation of regular opal structures from spherical silica particles in various colloidal solutions

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Abstract

Photonic crystal opal matrices are bulk spatial periodic structures based on amorphous spherical silica particles whose size is compatible with the wavelengths of the visible light spectrum. These structures are very promising and can be used as matrices for new functional materials.

The article studies the formation of a regular opal structure on dielectric substrates by means of the evaporation of droplets and layers of colloidal solutions based on water and ethanol with various concentrations of spherical SiO₂ particles with a diameter of about 250 nm synthesised using the Stöber method.

Keywords: Opal structures, Evaporation-induced self-assembly method, Tetraethoxysilane, Sedimentation, Lyophilic medium, Iridescence

Research article

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Effect of the morphology and composition of trimetallic PtCuAu/C catalysts on the activity and stability of the methanol oxidation reaction

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Abstract

A study on the influence of the method for obtaining trimetallic PtCuAu/C catalysts on their activity in the oxidation of methanol has been carried out.

The structural characteristics of the obtained trimetallic catalysts have been studied by X-ray diffraction and transmission electron microscopy. The nanoparticles of the material obtained by the galvanic synthesis method had a size twice as large (~ 6 nm) than the nanoparticles of the material obtained by the co-deposition of metal precursors. According to the results from the accelerated stress testing of catalysts, it was found that the material obtained by the galvanic method of substitution of copper atoms with gold had a higher residual activity in the oxidation of methanol than the commercial Pt/C analogue.

This study shows the potential of obtaining and using multicomponent platinum-containing nanoparticles deposited on a carbon carrier as effective catalysts for use in methanol fuel cells.

Keywords: methanol fuel cells, catalysis, trimetallic catalysts, galvanic replacement

Research article

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The kinetics of cathodic hydrogen evolution on titanium disilicide in a sulphuric acid solution

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Abstract

The kinetics and mechanism of hydrogen evolution reaction on the TiSi₂ electrode in x M H₂SO₄ + (0.5 - x) M Na₂SO₄ (x = 0.5; 0.35; 0.20; 0.05) solutions were studied using the methods of polarisation and impedance measurements.

The cathodic polarisation curves of TiSi₂ were characterised by a Tafel section with a slope of 0.116–0.120 V at E ranging from –0.30 to –0.48 V (SHE). The value of hydrogen evolution overpotential at $i = 1$ A/cm² for TiSi₂ was 0.90–0.96 V. The kinetic parameters of the hydrogen evolution reaction on silicide were close to the theoretical values for the slow stage of charge transfer.

Based on the measurements of the differential capacitance of the TiSi₂ electrode (at $f = 10$ kHz), depending on the cathodic polarisation and acidity of the electrolyte, it was concluded that a thin dielectric film of silicon dioxide (Si + 2H₂O → SiO₂ + 4H⁺ + 4e⁻) was present on the surface of the silicide. The film was not reduced with low cathodic polarisations.

The impedance spectra of the TiSi₂ electrode at the potentials of the Tafel region were capacitive semicircles with a misplaced centre. The impedance spectra were described by an equivalent electrical circuit, the Faraday impedance of which consisted of a series-connected charge transfer resistance R_1 and a parallel R_2C_2 chain corresponding to the adsorption of atomic hydrogen on the electrode surface. The impedance of the double layer capacitance was modelled using the constant phase element CPE₁. The χ^2 criterion for the circuit was (1.3–3.7)·10⁻⁴ (when

using data modulus weighting), the sum of square deviations was $(1.5–4.1) \cdot 10^{-2}$, and the error in the determination of the values of circuit parameters did not exceed 10 %.

The experimental values of the slopes of $\lg R_{1,E}$, $\lg R_{2,E}$, and $\lg C_{2,E}$ -dependences were close to the theoretical values of the slopes for the discharge-electrochemical desorption mechanism, in which both stages were irreversible and the transfer coefficients of the stages were not equal, when the Langmuir isotherm for adsorbed atomic hydrogen was fulfilled. The reaction of absorption of hydrogen with the kinetic control proceeded at the same time as the hydrogen evolution reaction.

Keywords: titanium disilicide TiSi_2 , hydrogen evolution reaction, sulphuric acid solution, impedance

Research article

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Effect of ethanol vapour sorption on the semiconductor-metal phase transition in powdered vanadium dioxide

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Abstract

We studied the effect of ethanol vapour on the parameters of the semiconductor-metal transition in a polycrystalline vanadium dioxide powder of the stable monoclinic phase $\alpha\text{-VO}_2$. It was synthesised by reducing vanadium pentoxide with oxalic acid while heated in air. The DC electrical resistance of the samples was studied between room temperature and 100 °C in a tubular heater, in a microcompressor-generated air stream with saturated ethyl alcohol vapour. It was found that in the presence of ethanol vapour, the hysteresis loop shifted to higher temperatures by ten degrees and its cooling branch (corresponding to the transition of vanadium dioxide from the metallic phase to the semiconductor phase) became stepped.

Keywords: Vanadium dioxide, Semiconductor - metal phase transition, Ethanol vapour, Sorption

Research article

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Polycondensation in a spray of aqueous-alcoholic solution of lactic acid

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Abstract

The removal of low molecular weight products of the reaction and heat withdrawal is one of the problems of bulk polycondensation. Polycondensation under spray conditions is an effective way to solve these problems.

Based on the example of the reversible reaction of lactic acid polycondensation, it was shown that size effects can significantly affect the conversion rate, the degree of polymerization, and the rate of processes. Chemical thermodynamics suggests that chemical equilibrium in a spray shifts towards the formation of polylactide. In addition, the recondensation of volatile components (water, lactic acid, solvent) stabilizes the concentration of reagents and the temperature in the spray drops throughout the entire process. Model experiments confirming the obtained regularities are presented. Microscopic observation of sessile drops of aqueous and aqueous-alcoholic lactic acid solutions demonstrated the formation of polylactide under normal conditions (without heating, catalyst, evacuation).

The described regularities are of a thermodynamic nature and are relevant for polymerization and polycondensation processes involving volatile monomers and solvents.

Keywords: Polycondensation, Spray, Polylactide, Microencapsulation, Phase transitions

Research article

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Structural and magnetic properties of Ho-doped CuFe_2O_4 nanoparticles prepared by a simple co-precipitation method

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Abstract

Nanocrystalline copper (II) ferrite with a spinel structure doped with holmium was synthesized by co-precipitation using an aqueous solution of NaOH as a precipitant and subsequent annealing at 800 °C for 60 min. The doping limit was determined by X-ray phase analysis. The similarity of the real and nominal compositions of the doped samples was established by energy-dispersive X-ray spectroscopy using a scanning electron microscope. The obtained particles had an approximately spherical shape, and their size was 40–70 nm (X-ray phase analysis, transmission electron microscopy). The introduction of Ho^{3+} cations to $x = 0.15$ into a CuFe_2O_4 spinel lattice led to a decrease in the average size of crystallites, an increase in the coercive force of nanopowders, and a decrease in excess magnetization and saturation magnetization. Synthesized $\text{CuFe}_{2-x}\text{Ho}_x\text{O}_4$ ($x = 0, 0.1$ and 0.15) nanopowders were magnetically hard materials with high coercive force.

Keywords: CuFe_2O_4 , Ho-doping, Co-precipitation method, Magnetic properties

Research article

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Investigation of the effect of a multicomponent additive on the structure formation and hardening of cement composites

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Abstract

The development and application of multicomponent multifunctional additives for cement composites is an important research area since the use of such additives allows controlling both the rheological properties of the freshly prepared mixture and the physical and mechanical characteristics of the finished composite.

This work proposes to use a multicomponent multifunctional additive with the composition of “SiO₂ nanoparticle - superplasticiser - polypropylene fibre” for the modification of cement composite materials based on sand and chalky flour. We studied the peculiarities of the influence of this additive on the technological characteristics of mixtures (plasticity and form stability) and the processes of setting-up, hydration, structure formation, and strength gain of the composite materials.

It was shown that the introduction of this additive allows increasing the plasticity limit and structural strength and reducing relative plastic deformations of the cement mixture at the manufacturing stage. At the same time, this additive accelerates the processes of setting-up, hydration, and strength gain of cement composites. It was proved that the increase in strength is due to the formation of a dense structure of hydrated new growths of the cement substance formed by phases of low and highly basic calcium silicate hydrates of various compositions and morphologies, as well as the absence of a portlandite phase.

The optimal ratio of indicators of plasticity and form stability of cement mixtures and the strength of composites based on them obtained by using the studied additive allows us to recommend to use this additive in the innovative construction 3D printing technology.

Keywords: Cement hardening systems, Modification, Structure formation, Multifunctional additives, Rheological characteristics, Compressive strength

Research article

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A model of interdiffusion occurring during the formation of thin metal films on single-crystal silicon under conditions of limited solubility of the components

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Abstract

Thin metal films are used in semiconductor and microelectronic devices to form ohmic and non-ohmic contacts to single-crystal silicon. A common feature of the used Me–Si systems is the low mutual solubility of elements and the polycrystalline nature of metal films. Solid-phase interactions during the deposition of metals on single-crystal silicon and the subsequent vacuum annealing results in the redistribution of the elements near the Me/Si interface. An important task facing the material science of solid-state electronics is to develop a mechanism of solid-phase interaction of metal thin films and single-crystal silicon. The aim of our study – was to develop a quantitative model of interdiffusion in the Me–Si system under conditions of limited solubility of the components.

The article suggests a mechanism of formation of Me–Si systems based on the diffusion and segregation of silicon near the intergrain boundaries of the metal and the limited formation of complexes during the diffusion-induced penetration of metal into silicon. The article suggests a model of reactive interdiffusion in thin metal film – single-crystal silicon systems under conditions of limited solubility of the components. Mathematical modelling was used to study the interaction of magnetron-sputtered metals Ti, W, and Nb with single-crystal silicon during isothermal vacuum annealing. The numerical analysis of experimental distributions of concentrations of Me and Si obtained by Rutherford backscattering spectroscopy allowed us to determine their individual diffusion coefficients in Me–Si systems.

The model can be used for empirical studies of the redistribution of the elements of two-layer systems with limited solubility, as well as to forecast the technological conditions for the production of electronic devices.

Keywords: Modelling, Reactive interdiffusion, Limited solubility, Metal thin films, Single-crystal silicon.