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### Аннотации на английском языке

Review

Review article https://doi.org/10.17308/kcmf.2021.23/3427

### Zirconium dioxide. Review

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#### Abstract

A review of zirconium dioxide or zirconia  $ZrO_2$  is presented. The finding of zirconium compounds in nature, the physical and chemical properties of  $ZrO_2$  are given, the polymorphism of zirconium oxide, and the phase diagrams of systems with its participation are considered. The areas of application of zirconia compounds are highlighted: automotive industry, electronics industry, energy and industrial ecology, equipment manufacturing and mechanical engineering the production of zirconium-based refractories, ceramics, enamels, glass, superhard materials, applications in medicine, nuclear energetics, and many others areas of human activity. Cubic modification of zirconium dioxide, stabilized by oxides of rare earth elements, is a jewelry stone (fianite). Partially stabilized zirconium dioxide is a versatile structural material with very high resistance to crack propagation. Solid solutions of REE oxides, especially scandium, have a high oxygen conductivity, which is used in sensors for measuring the partial pressure of oxygen and in fuel cells. Attention is paid to heat-resistant oxide ceramic materials with low thermal conductivity used in the quality of heat-resistant coatings. Considerable attention was paid to the second most important mineral of zirconia - baddeleyite ( $ZrO_2$ ). Baddeleyite is widely used in the production of refractory materials. It is mined for the production of metallic zirconium. The achievements of Soviet and Russian scientists in the development of technologies for the production of fianite and artificial baddeleyite are presented.

**Keywords**: Fianite, Baddeleyite, Zircon, Ceramics, Solid solutions, Oxides of rare earth elements, Phase diagrams, Inert matrix nuclear fuel

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# Condensed Matter and Interphases

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3428

# Study of the formation of structures in solutions of chitosan – polyvinyl alcohol polymer blends

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#### Abstract

The aim of this work was the investigation of the formation of structures in solutions of individual polymers, as well as their blends with each other in buffer solvents with different values of pH. In this study we used a sample of chitosan (degree of deacetylation ~ 84 %, M = 130,000), which is a polycation when dissolved, and polyvinyl alcohol ( $\rho$  = 1.25 g/cm<sup>3</sup>, M = 5000). Buffer systems based on acetic acid and sodium acetate with pH = 3.8, 4.25, and 4.75 were used as solvents. Viscosimetry was used to determine the intrinsic viscosity, the degree of structuring, and the Huggins constant. The Kriegbaum method was used to determine the nature of the aggregates formed by the blend of the studied polymers.

In the course of the research, it was shown that an increase in the pH of the acetate buffer used as a solvent was accompanied by a compression of the macromolecular coil (a decrease in intrinsic viscosity values), a deterioration in the quality of the solvent (an increase in Huggins constant values), and an increase in the degree of polymer aggregation in a solution for chitosan polyelectrolyte. At the same time for a solution of polyvinyl alcohol the pH of the buffer practically did not affect the nature of the polymer-solvent interaction. It has been proved that polymer blends are characterized by an increase in aggregation processes and a decrease in the thermodynamic quality of the solvent in comparison with solutions of individual polymers. The size of the "combined" macromolecular coil, characterized by the intrinsic viscosity value for the polymer blend, which can be both above (buffer solvent with pH = 3.80) and below (buffer solvent with pH = 4.25 and 4.75) additive values, changed depending on the type of formed polymer-polymer aggregates (homo- or hetero-). It was established that the type of aggregates (homo- or hetero-) formed in solutions of polymer blends was determined not only by the thermodynamic quality of the used solvents, but also by the concentration of the polymers in the initial solutions.

Keywords: Polymer blends, Viscometry, Structure formation, Chitosan, Polyvinyl alcohol

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3429

# Sol-gel synthesis, crystal structure and magnetic properties of nanocrystalline praseodymium orthoferrite

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### Abstract

In this work, nano-sized crystalline praseodymium orthoferrite was successfully synthesized via sol-gel method using water – methanol co-solvent. Single-phase  $PrFeO_3$  nanoparticles were formed after annealing the precursors at 650, 750, 850, and 950 °C during 60 min. The crystal size, lattice volume and coercivity ( $H_c$ ) of nanocrystalline  $PrFeO_3$  increase with the annealing temperature. The obtained praseodymium orthoferrite exhibited paramagnetic properties with  $H_c = 28 - 34$  Oe.

Keywords: Sol-gel synthesis, Methanol, Praseodymium orthoferrite, Magnetic property

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3430

### Growing epitaxial layers of InP/InGaAsP heterostructures on the profiled InP surfaces by liquid-phase epitaxy

### M. G. Vasil'ev<sup>\varsil'</sup>, A. M. Vasil'ev, A. D. Izotov<sup>\varsil'</sup>, Yu. O. Kostin, A. A. Shelyakin

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#### Abstract

The effect of various planes was studied when growing epitaxial layers by liquid-phase epitaxy (LPE) on the profiled InP substrates. The studies allowed obtaining buried heterostructures in the InP/InGaAsP system and creating highly efficient laser diodes and image sensors.

It was found that protruding mesa strips or in-depth mesa strips in the form of channels formed by the {111}A, {111}B, {110}, {112}A, or {221}A family of planes can be obtained with the corresponding selection of an etching agent, strip orientation, and a method of obtaining a masking coating. It was noted that in the case of the polarity of axes being in the direction of <111>, the cut of mesa strips was conducted along the most densely packaged planes. This cut led to the difference in rates of both chemical etching and epitaxial burying of profiled surfaces.

The cut was made along the planes at a low dissolution rate  $\{111\}A$  for a sphalerite lattice, to which the studied material, indium phosphide, belongs. Analysis of planes  $\{110\}$  and  $\{\overline{I}10\}$  showed that the location of the most densely packaged planes  $\{111\}A$  and  $\{111\}B$  relative to them is different.

Keywords: Heterostructures, Laser diodes, Indium phosphide, Buried heterostructures, Channel in the substrate

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# Condensed Matter and Interphases

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3431

### Anomalous behaviour of dynamic electrical conductivity in semiconductor ferroelectric ceramics near the phase transition temperature

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### Abstract

The article presents the results of a study of the electrical properties of semiconductor perovskite ceramics based on a solid solution of barium-strontium titanate with the addition of the rare earth element of cerium with the initial formula  $Ba_{1-x-y}Sr_xCe_yTiO_3$  (x = 0.05, y = 0.003). A scanning electron microscope was used to obtain images of the sample surfaces and the elemental composition data. The measurements were performed by impedance spectroscopy in the temperature range of 348-385 K in the frequency range of  $10^2-10^6$  Hz using an LCR metre. It was found that there is an anomalous behaviour in the dynamic electrical conductivity of the samples in the temperature range close to the ferroelectric-paraelectric phase transition. This is expressed by a decrease in the value of the real part of the dynamic conductivity with an increase in frequency. An analysis of the simplified equivalent circuit of the intergranular barrier showed that this anomaly can be explained by introducing an inductive element into the circuit. This element can be considered a "negative capacitance element". Following the results of the study, a conclusion was made about the generalised character of the phenomenon.

Keywords: Semiconductor ceramics, Impedance spectroscopy, Negative capacitance effect, Posistor

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3432

# On the limitations of the applicability of Young's equations temperature

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### Abstract

The article uses the thermodynamics of interfacial phenomena to justify the fact that Young's equations can correctly describe the three-phase equilibrium with any type of interatomic bonds.

Wetting, adhesion, dissolution, surface adsorption, and other surface phenomena are important characteristics, which largely determine the quality and durability of materials, and the development of a number of production techniques, including welding, soldering, baking of metallic and non-metallic powders, etc. Therefore, it is important to study them.

Using experimental data regarding surface energies of liquids (melts) and contact angles available in the literature, we calculated the surface energies of many solid metals, oxides, carbides, and other inorganic and organic materials without taking into account the amount of the interfacial energy at the solid-liquid (melt) interface. Some researchers assumed that in case of an acute contact angle the interfacial energy is low. Therefore, they neglected it and assumed it to be zero. Others knew that this value could not be measured, that is why they measured and calculated the difference between the surface energy of a solid and the interfacial energy of a solid and a liquid (melt), which is equal to the product of the surface energy of this liquid by the cosine of the contact angle. It is obvious that these methods of determining the surface energy based on such oversimplified assumptions result in poor accuracy.

Through the use of examples this paper shows how the surface energies of solids were previously calculated and how the shortcomings of previous calculations can be corrected.

Keywords: Surface energy, Interfacial energy, Wetting angle, Nickel, Cobalt, Graphite, Titanium carbide

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3433

### The structure of carbon nanotubes in a polymer matrix

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#### Abstract

We carried out an analytical structural analysis of interfacial effects and differences in the reinforcing ability of carbon nanotubes for polydicyclopentadiene/carbon nanotube nanocomposites with elastomeric and glassy matrices. In general, it showed that the reinforcing (strengthening) element of the structure of polymer nanocomposites is a combination of the nanofiller and interfacial regions. In the polymer matrix of the nanocomposite, carbon nanotubes form ring-like structures. Their radius depends heavily on the volume content of the nanofiller. Therefore, the structural reinforcing element of polymer/carbon nanotube nanocomposites can be considered as ring-like formations of carbon nanotubes coated with an interfacial layer. Their structure and properties differ from the characteristics of the bulk polymer matrix. According to this definition, the effective radius of the ring-like formations increases by the thickness of the interfacial layer. In turn, the level of interfacial adhesion between the polymer matrix and the nanofiller is uniquely determined by the radius of the specified carbon nanotube formations. For the considered nanocomposites, the elastomeric matrix has a higher degree of reinforcement compared to the glassy matrix, due to the thicker interfacial layer. It was shown that the ring-like nanotube formations could be successfully modelled as a structural analogue of macromolecular coils of branched polymers. This makes it possible to assess the effective (true) level of anisotropy of this nanofiller in the polymer matrix of the nanocomposite. When the nanofiller content is constant, this level, characterised by the aspect ratio of the nanotubes, uniquely determines the degree of reinforcement of the nanocomposites.

Keywords: Nanocomposite, Carbon nanotubes, Structure, Interfacial layer, Ring-like formations, Reinforcement degree

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3434

# Features of the discharge of zinc in the background solution of sodium sulphate under stirring conditions

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#### Abstract

The production technology of hydrometallurgical zinc uses various surfactants to thicken pulps, stabilise the electrolysis process, and obtain high-quality cathode deposits. Numerous researches were conducted to study the cathodic and anodic processes in a wide range of the composition of aqueous solutions using various solid electrodes in the absence of intense stirring of the electrolyte and with a high contribution of the migration component of the discharge of metals. This approach to the study of the surfactants' influence rarely provided a high degree of statistical reliability in observing the effect of differently charged surfactants on electrode processes, which is of great importance in the hydrometallurgical production of zinc. In this work, the task was to practically eliminate the contribution of the migration component due to the following factors: conducting electrolysis in a background solution of sodium sulphate, organising electrolyte stirring, performing calculations of current densities at the beginning of electrolysis, and establishing polarisation curves at an increased potential sweep rate from 20 to 100 mV/s. This approach provided a greater degree of statistical reliability in presenting the mechanism of the effect of additions of cationic and anionic surfactants during the stage of zinc discharge on a solid electrode, which was the purpose of the article.

Electrolysis was conducted in the potential range from -1050 to -1250 mV relative to the silver chloride electrode (AgCl/Ag) in the presence of a background sodium sulphate solution (0.5 M of  $Na_2SO_4$  solution) containing 0.005, 0.0125, and 0.025 M ZnSO4 with the introduction of high-molecular surfactants: cationic and anionic coagulants (flocculants) and foaming agents (lignosulphonate – LSTP).

During the electrolysis in a background solution of sodium sulphate with stirring, it was found that the process of discharge of zinc ions on a solid electrode occurs in a mixed-kinetic mode. It was shown that positively charged additives, such as lignosulphonate and cationic coagulant (flocculant) Besfloc K6645, have a negative effect on the dynamics of zinc cation discharge, while negatively charged Besfloc K4034 has practically no effect. The approach proposed in this work allows evaluating the influence of additions of cationic and anionic surfactants on the stage of zinc discharge on a solid electrode, which was the practical and scientific value of this work.

Keywords: Zinc, Current density, Potential, Polarisation, Coagulant, Lignosulphonate, Sodium sulphate, Electrode

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### Condensed Matter and Interphases

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3435

# Phase relations in the CuI-SbSI-SbI<sub>3</sub> composition range of the Cu–Sb–S–I quaternary system

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### Abstract

The phase equilibria in the Cu-Sb-S-I quaternary system were studied by differential thermal analysis and X-ray phase analysis methods in the CuI-SbSI-SbI<sub>3</sub> concentration intervals. The boundary quasi-binary section CuI-SbSI, 2 internal polythermal sections of the phase diagram, as well as, the projection of the liquidus surface were constructed. Primary crystallisation areas of phases, types, and coordinates of non- and monovariant equilibria were determined. Limited areas of solid solutions based on the SbSI ( $\beta$ -phase) and high-temperature modifications of the CuI ( $\alpha_1$ - and  $\alpha_2$ - phases) were revealed in the system. The formation of the  $\alpha_1$  and  $\alpha_2$  phases is accompanied by a decrease in the temperatures of the polymorphic transitions of CuI and the establishment of metatectic (375°C) and eutectoid (280°C) reactions. It was also shown, that the system is characterised by the presence of a wide immiscibility region that covers a significant part of the liquidus surface of the CuI and SbSI based phases.

**Keywords:** Copper (I) iodide, Antimony iodide, Antimony sulfoiodide, Cu-Sb-S-I system, Phase diagram, Solid solutions *Acknowledgements:* the work has been partially supported by the Science Development Foundation under the President of the Republic of Azerbaijan, a grant N<sup>o</sup> EİF-BGM-4-RFTF-1/2017-21/11/4-M-12.

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# Condensed Matter and Interphases

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3436

### Gender differences in lipid metabolism

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### Abstract

The search for early markers of atherosclerosis is an effective method for providing personalized medicine allowing the prevention of the progression of this pathology. The aim of this study was the determination of the total indices of dyslipidemia and the identification of the gender indices of the extended lipid profile in the population of residents of the Southern and Central Federal Districts (Voronezh, Belgorod, Lipetsk, Kursk and Rostov regions) for the identification of early markers of atherogenicity. In a simultaneous clinical study, involving 339 patients (mean age 48 years), the concentrations of total cholesterol, triglycerides, LDL (low density lipoproteins), HDL (high density lipoproteins), apolipoproteins B and A1, the ApoB/ApoA1 ratio and the atherogenic coefficient were determined. For the identification of the relationship between changes in lipid profile indicators with cytolysis syndrome and indicators of carbohydrate metabolism, the activity of ALAT (alanine aminotransferase), GGTP (gamma-glutamyl transpeptidase) and glucose content were also studied. Analysis of the results of the lipid spectrum of the population sample of the middle age group revealed significant metabolic disorders of lipid fractions in middle-aged men in comparison with women. It has been shown that the apoB/apoA1 index can be used as an auxiliary marker for early assessment of the prevalence of atherogenic lipid fractions, allowing the identification of risk groups for the development of diseases associated with metabolic disorders.

**Keywords:** Lipid metabolism, Atherosclerosis, Metabolic syndrome, Cholesterol, Triglycerides, LDL, HDL, ApoV / ApoA1, Atherogenic coefficient

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![](_page_10_Picture_6.jpeg)

### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3437

### Heat wave dynamics in frozen water droplets with eosin molecules under the femtosecond excitation of a supercontinuum

N. A. Myslitskaya<sup>1,2<sup>IZ</sup></sup>, A. V. Tcibulnikova<sup>1</sup>, I. G. Samusev<sup>1</sup>, V. A. Slezhkin<sup>1,2</sup>, V. V. Bryukhanov<sup>1</sup>

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### Abstract

In this study, we considered thermal processes in liquid and frozen water droplets with added dye molecules and metal nanoparticles at the moment of supercontinuum generation. We studied optical non-linear processes in a water droplet with a diameter of 1.92 mm, cooled (+2 °C) and frozen to -17 °C, with eosin molecules and ablative silver nanoparticles upon femtosecond laser treatment.

When we exposed a cooled water droplet and a piece of ice containing eosin molecules and ablative silver nanoparticles to a femtosecond laser beam ( $\lambda = 1030$  nm), we recorded two-photon fluorescence, enhanced by plasmon processes. Also, supercontinuum generation took place, with a period of decay t = 0.02 s. The geometry of non-linear large-scale self-focusing ( $L_{LSS} \sim 0.45-0.55$  mm) was studied. The value of microscale self-focusing ( $L_{SSS} \sim 0.1$  mm) of SC radiation in the laser channel was determined experimentally. The study shows that the energy dissipation in the SC channel increases when the thermal non-linearity exceeds the electronic non-linearity. We modelled the thermal processes and determined the temperature gradient of the heating of the frozen droplet exposed to a femtosecond pulse. Based on the experimental data, the heat wave propagation velocity was calculated to be v = 0.11 m/s.

**Keywords:** Supercontinuum, Femtosecond excitation, Water, piece of ice, Eosin fluorescence, Ablative silver nanoparticles, Surface plasmons, Two-photon excitation, Thermal optical non-linearity, Temperature gradient, Heat wave, Wave propagation velocity

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![](_page_12_Picture_2.jpeg)

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## Condensed Matter and Interphases

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**Original articles** 

Research article https://doi.org/10.17308/kcmf.2021.23/3438

### Thermodynamic study of manganese tellurides by the electromotive force method

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### Abstract

The thermodynamic properties of manganese tellurides were determined using an electromotive force (EMF) method with a liquid electrolyte in a temperature range from 300 to 450 K. EMF measurements were performed using equilibrium samples taken from the two-phase regions, namely  $MnTe_2$  + Te and  $MnTe + MnTe_2$ , of the Mn–Te system. The phase compositions of all samples were controlled with the X-ray diffraction (XRD) method. The partial molar functions of manganese in alloys, as well as the standard thermodynamic functions of the formation and standard entropies of MnTe and  $MnTe_2$ , were calculated. A comparative analysis of obtained results with literature data is performed.

**Keywords:** Electromotive force method, Thermodynamic properties, Manganese tellurides, MnTe, MnTe<sub>2</sub>, Partial molar functions

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### **Original articles**

Research article https://doi.org/10.17308/kcmf.2021.23/3478

### Electrophilic-nucleophilic properties as a factor in the formation of antifriction and hydrophobic properties of surface-modified metals with ammonium and organosilicon compounds

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#### Abstract

Stabilisation of the functional properties of dispersed and compact metals, as well as the regulation of their reactivity, improvement of water-repellent, antifriction and anti-corrosion properties by creating the protective films on the surface is an urgent problem in relation to obtaining new materials. Previously, research conducted at REC "Nanotechnology" of the St. Petersburg Mining University proved that chemisorption of ethylhydridesiloxane vapours together with surfactants based on quaternary ammonium compounds has a beneficial effect on the water-repellent properties of metals. In order to obtain the physicochemical mechanism of the hydrophobisation of the surface of modified dispersed metals for the first time, the study of the electrophilic-nucleophilic properties of the active substances of the surface modifiers of metals was carried out using the methods of quantum-chemical modelling using HyperChem software package. The dipole moment, energy of the highest occupied and the lowest unoccupied molecular orbitals, electrophilic-nucleophilic properties were determined. The series of enhancement of nucleophilic/electrophilic properties and dipole moment for modifiers were obtained. The donor-acceptor properties, the differences in the characteristics of the molecules of alkamon, triamon, and hydrophobic silicone organic liquid were quantitatively and qualitatively established. The regularities of the formation of hydrophobic and antifiction properties in the composition of industrial oil I-20-surface-modified metal with various electrophilic-nucleophilic properties of the applied substances.

**Keywords:** Electrophilic-nucleophilic properties, Dispersed metals, Ethylhydridesiloxane oligomer, Quantum-chemical modelling, Hydrophobicity, Antifriction properties

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