

ISSN 1606-867X (Print) ISSN 2687-0711 (Online)

Конденсированные среды и межфазные границы

https://journals.vsu.ru/kcmf/

Аннотации на английском языке

Review

Review article

https://doi.org/10.17308/kcmf.2023.25/11256

Preparation, luminescence, and application of LiMeBO₃ borates, Me = Mg, Ca, Sr, Ba, Zn, Cd. Review T. N. Khamaganova

Baikal Institute of Nature Management Siberian Branch of the Russian Academy of sciences 6 Sakhyanovoy st., Ulan-Ude, Buryatia, Russian Federation

Abstract

The review summarises and analyses data on the preparation, structure, and spectral-luminescent properties of $LiMeBO_3$ -based borates, Me = bivalent metal.

These polycrystalline borates are prepared traditionally by solid-phase reactions and self-propagating high-temperature synthesis and its modifications based on a combustion reaction.

Frameworks of lithium borates with alkaline earth metals, zinc, and cadmium are formed from large metal polyhedra between which there are boron-oxygen triangles isolated from each other. Doping with rare-earth and heavy metal ions leads to the formation of solid solutions which normally have defective structures. Doped activator ions often become the main part of the luminescence centre in the phosphor. The luminescent properties of ions of rare-earth elements arise from the possibility of electronic transitions between states within the 4f-configuration. The paper discusses the most likely mechanisms of charge compensation during heterovalent substitution in LiMeBO₃ borates (co-doping and formation of cation vacancies). It is shown that charge compensation during the combined introduction of ions of REEs and alkali metals into the structure has a positive effect on the emission yield. The review considers the results of thermoluminescent, upconversion, and photoluminescent properties and processes and phenomena that cause them. It also explains the mechanism of resonance energy transfer from the sensitiser to the activator using the example of $Yb^{5r} \rightarrow Er^{5r}$.

It discusses the possibility of using the considered borates as phosphors that emit green, blue, and red light in white LEDs and as effective materials for personnel neutron dosimetry and the dosimetry of weak ionising radiation.

Keywords: Polycrystalline borates, Solid-phase synthesis, Combustion method, LEDs, Thermoluminescence, Green phosphor, Sensitisation *Funding:* The study was supported by the Ministry of Science and Higher Education of the Russian Federation (the government order to the Baikal Institute of Nature Management, Siberian Branch of the Russian Academy of Sciences, project No. 0273–2021-0008).

For citation: Khamaganova T. N. Preparation, luminescence, and application of LiMeBO₃ borates, Me= Mg, Ca, Sr, Ba, Zn, Cd. Review. *Condensed Matter and Interphases.* 2023;25(3): 311–332. https://doi.org/10.17308/kcmf.2023.25/11256

Original articles

Research article

https://doi.org/10.17308/kcmf.2023.25/11311

Interdiffusion in the formation of thin niobium films on single-crystal silicon under vacuum annealing conditions N. N. Afonin¹, V. A. Logacheva²

¹Voronezh State Pedagogical University,

86 ul. Lenina, Voronezh 394043, Russian Federation

²Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

Abstract

For the design of technological process for creating device structures based on niobium and single-crystal silicon with the desired properties, empirical and theoretical knowledge about the solid-phase interaction process in the system of a thin niobium film is required. The purpose of the research was a comprehensive study of the redistribution of components during the formation of thin niobium films on single-crystal silicon obtained by magnetron-assisted sputtering followed by vacuum annealing.

The structure and phase composition were studied by X-ray phase analysis, scanning electron microscopy, and atomic force microscopy. Distribution of components along the depth was determined using the Rutherford backscattering spectrometry.

The traditional experimental method for studying the process of interdiffusion of components in binary macroscopic systems is the placing of inert marks. However, the use of this method in systems containing thin films is hindered by the comparable thicknesses of the films and marks. This circumstance makes the mathematical modelling the most convenient method for the analysis of the interdiffusion process in thin-film systems.

The interdiffusion model during the formation of polycrystalline niobium film – single-crystal silicon systems, developing the Darken's theory for the limited solubility components was proposed. Grain boundary diffusion of silicon in the intergrain space of a polycrystalline niobium film was proposed. Numerical analysis of the experimental distribution of concentrations within the model established that silicon is the dominant diffusant in the studied system. The temperature dependence of the individual diffusion coefficient of silicon $D_{\rm si} = 3.0 \ 10^{-12} \exp(-0.216 \ {\rm eV}/(kT)) \ {\rm cm}^2/{\rm s}$ in the temperature range 423–773 K was determined.

The model is applicable to the description of the redistribution of components in the thin niobium film – single-crystal silicon system prior to synthesis conditions providing the chemical interaction of the metal with silicon and the formation of silicides. It illustrates the



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mechanism of the possible formation of silicide phases not by layer-by-layer growth at the Nb/Si grain boundary, but in its vicinity due to deep mutual diffusion of the components.

Keywords: Reactive interdiffusion, Limited solubility, Thin films, Niobium, Single-crystal silicon, Magnetron-assisted sputtering, Vacuum annealing, Rutherford backscattering spectrometry, Simulation method, Darken's theory

Acknowledgements: X-ray phase analysis and studied by atomic force microscopy were carried out using the equipment of the VSU Centre for Collective Use of Scientific Equipment https://ckp.vsu.ru/

For citation: Afonin N. N., Logacheva V. A. Interdiffusion in the formation of thin niobium films on single-crystal silicon under vacuum annealing conditions. *Condensed Matter and Interphases*. 2023;25(3): 333–342. https://doi.org/10.17308/kcmf.2023.25/11311

Research article

https://doi.org/10.17308/kcmf.2023.25/11257

Biocatalysts based on complexes of carbon nanomaterials with cysteine proteases

S. S. Goncharova¹, E. A. Shchegolevatykh¹, D. A. Zhukalin¹, M. G. Holyavka^{1,2}, V. G. Artyukhov¹

¹Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

²Sevastopol State University,

33 Universitetskaya str., Sevastopol 299053, Russian Federation

Abstract

The purpose of the research is to develop and study biocatalysts based on complexes of cysteine proteases with fullerenes and carbon nanotubes.

During the formation of ficin complexes with fullerenes and carbon nanotubes, the activity of hybrid preparations was 70 and 45%, respectively. During the formation of papain complexes with fullerenes and carbon nanotubes, the proteolytic ability of the enzyme remained at the same level for the samples with fullerene and decreased by 27% for the preparations with carbon nanotubes. The formation of bromelain complexes with fullerenes and carbon nanotubes contributed to a decrease in the proteolytic activity of the biocatalyst by 18 and 48% as compared to the free enzyme. While determining the stability of complexes of nanomaterials and cysteine proteases during a 7-day incubation in 0.05 M tris-HCl buffer (pH 7.5) at 37 °C, we noticed a decrease in the proteolytic activity of the samples.

Complexation with carbon nanoparticles and fullerenes increased the stability of ficin and bromelain, while the stability of papain in the complexes remained unchanged.

Keywords: Cysteine proteases, Ficin, Papain, Bromelain, Fullerenes, Carbon nanotubes

Acknowledgements: The research was funded by the Ministry of Science and Higher Education of the Russian Federation in the framework of the government order to higher education institutions in the sphere of scientific research for years 2023-2025, project No. FZGU-2023-0009.

For citation: Goncharova S. S., Shchegolevatykh E. A., Zhukalin D. A., Holyavka M. G., Artyukhov V. G. Biocatalysts based on complexes of carbon nanomaterials with cysteine proteases. *Condensed Matter and Interphases*. 2023;25(3): 343–349. https://doi.org/10.17308/kcmf.2023.25/11257

Research article

https://doi.org/10.17308/kcmf.2023.25/11258

Formation of plasmon-exciton nanostructures based on quantum dots and metal nanoparticles with a nonlinear optical response

A. I. Zvyagin, T. A. Chevychelova, A. S. Perepelitsa, M. S. Smirnov, O. V. Ovchinnikov

Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

Abstract

The establishment of the conditions for the formation of nanostructures with plasmon-exciton interaction based on quantum dots and plasmonic nanoparticles that provide unique nonlinear optical properties is an urgent task. The study demonstrates the formation of plasmon-exciton nanostructures based on hydrophilic colloidal $Zn_0 Cd_0 SAg_2$ quantum dots and metal nanoparticles.

Transmission electron microscopy and optical absorption and luminescence spectroscopy were used to substantiate the formation of plasmon-exciton hybrid nanostructures. The phase composition of the studied samples was determined by X-ray diffraction. The results obtained using ARLX'TRA diffractometer (Switzerland) indicated a cubic crystal structure (F43m) of synthesised $Zn_{0.5}Cd_{0.5}S$ quantum dots and monoclinic ($P2_1/C$) crystal lattice of Ag₂S. Transmission electron microscopy revealed that plasmonic nanoparticles are adsorption centres for quantum dots. The average sizes of the studied samples were determined: colloidal Ag₂S quantum dots (2.6 nm), $Zn_{0.5}Cd_{0.5}S(2.0 nm)$ and metal nanoparticles: silver nanospheres (10 nm) and gold nanorods (4x25 nm). The transformation of the extinction spectra of the light and the luminescence quenching of quantum dots have been established in mixtures of quantum dots and plasmonic nanoparticles. The nonlinear optical parameters of the studied samples were determined using the Z-scanning method at wavelengths of 355 and 532 nm in the field of nanosecond laser pulses. The conditions for the formation of hybrid nanostructures that provide an increase of the coefficient of nonlinear absorption of laser pulses (355 and 532 nm) up to 9 times with a duration of 10 ns due to the reverse saturable absorption occurring due to cascade two-quantum transitions in the intrinsic and local states of colloidal quantum dots and the suppression of nonlinear refraction, were determined.

The observed changes were explained by the manifestation of the Purcell effect on the states of quantum dots in the presence of nanoresonators (gold nanorods and silver nanospheres). The results of these studies create new opportunities for the development of original systems for controlling the intensity of laser radiation, as well as quantum sensors of a new generation.

Keywords: Nonlinear refraction, Nonlinear absorption, Quantum dot, Ag₂S, Zn_{0.5}Cd_{0.5}S, Plasmonic nanoparticle, Z-scan

Funding: The study was supported by the grant of the President of the Russian Federation No. MK-4408.2022.1.2

Acknowledgments: the study of structural properties by transmission electron microscopy and X-ray diffraction were carried out using the equipment of the VSU Centre for Collective Use of Scientific Equipment.

For citation: Zvyagin A. I., Chevychelova T. A., Perepelitsa A. S., Ovchinnikov O. V., Smirnov M. S. Formation of plasmon-exciton nanostructures based on quantum dots and metal nanoparticles with a nonlinear optical response. *Condensed Matter and Interphases*. 2023;25(3): 350–358. https://doi.org/10.17308/kcmf.2023.25/11258

Research article https://doi.org/10.17308/kcmf.2023.25/11259 Structure and composition of a composite of porous silicon with deposited copper A. S. Lenshin^{1,2}, K. B. Kim², B. L. Agapov¹, V. M. Kashkarov¹, A. N. Lukin¹, S. I. Niftaliyev² 'Voronezh State University, 1 Universitetskaya pl., Voronezh 394018, Russian Federation ²Voronezh State University of Engineering Technologies,

Revolution Avenue, 19, Voronezh 394036, Russian Federation

Abstract

Porous silicon is a promising nanomaterial for optoelectronics and sensorics, as it has a large specific surface area and is photoluminescent under visible light. The deposition of copper particles on the surface of porous silicon will greatly expand the range of applications of the resulting nanocomposites. Copper was chosen due to its low electrical resistivity and high resistance to electromigration compared to other metals. The purpose of this research was to study changes in the structure and composition of porous silicon after the chemical deposition of copper.

Porous silicon was obtained by the anodisation of monocrystalline silicon wafers KEF (100) (electronic-grade phosphorus-doped silicon) with an electrical resistivity of 0.2 Ohm-cm. An HF solution in isopropyl alcohol with the addition of H_2O_2 solution was used to etch the silicon wafers. The porosity of the samples was about 70 %. The porous silicon samples were immersed in copper sulphate solution (CuSO₄-5H₂O) for 7 days. We used scanning electron microscopy, IR spectroscopy, and ultrasoft X-ray emission spectroscopy to obtain data on the morphology and composition of the initial sample and the sample with deposited copper. The chemical deposition of copper on porous silicon showed a significant distortion of the pore shape as well as the formation of large cavities inside the porous layer. However, in the lower part the pore morphology remained the same as in the original sample. It was found that the chemical deposition of copper on porous silicon leads to copper penetrating into the porous layer, the formation of a composite structure, and it prevents the oxidation of the porous layer during storage. Thus, it was demonstrated that the chemical deposition of copper on a porous silicon surface leads to visible changes in the surface morphology and composition. Therefore, it should have a significant impact on the catalytic, electrical, and optical properties of the material. **Keywords:** Porous silicon, Composites, Copper, Ultrasoft X-ray emission Spectroscopy, Electronic structure

Funding: The study was supported by the Russian Foundation for Basic Research, project No. 22-73-0154.

For citation: Lenshin A. S., Kim K. B., Agapov B. L., Kashkarov V. M., Lukin A. N., Niftaliev S. I. Structure and composition of a composite of porous silicon with deposited copper. *Condensed Matter and Interphases*. 2023;25(3): 359–366. https://doi.org/10.17308/kcmf.2023.25/11259

Research article

https://doi.org/10.17308/kcmf.2023.25/11260

A study of the local atomic structure the environment of zinc ions of different concentrations during their interaction with the arachidic acid Langmuir monolayer

V. Yu. Lysenko¹, M. A. Kremennaya¹, S. N. Yakunin², A. V. Rogachev², G. E. Yalovega¹

¹Southern Federal University

105/42 Bolshaya Sadovaya st., Rostov-on-Don 344006, Russian Federation

²National Research Centre "Kurchatov Institute"

1 Academician Kurchatova pl., Moscow 123182, Russian Federation

Abstract

Vital cellular processes depend on the controlled transport of metal ions across biological membranes. A biological membrane is a complex system consisting of lipids and proteins, that is why simplified systems, in particular monomolecular layers, are used to model it.

This work presents the results of a study of the interaction of zinc ions from the aqueous subphase with the Langmuir monolayer of arachidic acid. The study was carried out for the first time and used total external reflection X-ray absorption spectroscopy. It considers the influence of the concentration of a ZnCl_2 aqueous subphase solution on the local environment of zinc ions when interacting with the lipid monolayer immediately after its formation.

The theoretical analysis of experimental XANES spectra showed that one of the interaction ways of arachidic acid molecules with zinc ions immediately after the monolayer formation is an intramolecular interaction with the formation of spodium bonds between the zinc cation and the OH carboxyl group of arachidic acid.

Keywords: arachidic acid, X-ray absorption spectroscopy, total external reflection, lipid layer, Langmuir bath, subphase, thin films *Funding:* The study was supported by the grant of the President of the Russian Federation (grant No. MK-2767.2021).

For citation: Lysenko V. Yu., Kremennaya M. A., Yakunin S. N., Rogachev A. V., Yalovega G. E. A study of the local atomic structure the environment of zinc ions of different concentrations during their interaction with the arachidic acid Langmuir monolayer. *Condensed Matter and Interphases.* 2023;25(3): 367–372. https://doi.org/10.17308/kcmf.2023.25/11260

Research article

https://doi.org/10.17308/kcmf.2023.25/11261

Hydrogen permeability of 48Cu52Pd cold-rolled alloy foil and different methods of its surface pretreatment N. B. Morozova¹, L. E. Sidyakina¹, A. I. Dontsov^{1,2}, A. V. Vvedenskii¹

¹Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

²Voronezh State Technical University,

20 letiya Oktyabrya st., 84, Voronezh 394006, Russian Federation

Abstract

The process of atomic hydrogen penetration into the metal phase is complicated by the phase-boundary transition from the liquid and/ or gas phase. That is why the cleanliness of metal and alloy surfaces is of particular importance. The purpose of this work was to determine the effect of surface pretreatment using photon pulses, ultrasound, and potential cycling on the parameters of hydrogen permeability for 48Cu52Pd metal cold-rolled membranes.

The study was focused on a foil of copper-palladium homogeneous alloy with 48 at. % Cu and 52 at. % Pd composition. The studied samples were obtained by cold rolling and their thickness were 10 and 16 µm. Surface pretreatment included rinsing in acetone, using ultrasound,

pulsed photon treatment, and quadruple potential cycling over a wide range of potentials. Electrochemical studies included cyclic voltammetry and cathode-anodic chronoamperometry in a deaerated $0.1 \text{ MH}_2\text{SO}_4$ solution. Hydrogen permeability was calculated using mathematical models for samples of finite and semi-infinite thickness.

It was found that the surface treatment of a 48Cu52Pd foil with photon pulses leads to both an increase in the ionisation rate of atomic hydrogen and an increase in the roughness of the foil surface. The diffusion coefficient of atomic hydrogen does not depend on the method of surface pretreatment with ultrasound and photon pulses. The extraction rate constant for the extraction of the atomic hydrogen after photon treatment increases, which facilitates the processes of both H introduction and ionisation due to the release of active centres of the surface. Electrochemical cleaning of the surface during the quadruple potential cycling contributes to the growth of the extraction rate constant for the extraction of atomic hydrogen.

Keywords: 48Cu52Pd foil, Cold rolling, Hydrogen permeability, Surface pretreatment, Pulsed photon treatment, Ultrasound

Funding: The work was supported by the Ministry of Science and Higher Education of the Russian Federation in the framework of the government order to higher education institutions in the sphere of scientific research for years 2023-2025, project No. FZGU-2023-0006. *For citation:* Morozova N. B., Sidyakina L. E., Dontsov A. I., Vvedenskii A. V. Hydrogen permeability of 48Cu52Pd cold-rolled alloy foil and different methods of its surface pretreatment. *Condensed Matter and Interphases*. 2023;25(3): 373–382. https://doi.org/10.17308/kcmf.2023.25/11261

Research article

https://doi.org/10.17308/kcmf.2023.25/11262

Composition and thermoelectric properties of structures based on iron silicide grown by pulse laser deposition

D. E. Nikolichev, R. N. Kriukov, A. V. Nezhdanov, A. V. Zdoroveyshchev, Yu. M. Kuznetsov, V. P. Lesnikov, D. A. Zdoroveyshchev, M. V. Dorokhin, P. B. Demina, A. A. Skrylev

Lobachevsky University,

23 Gagarin av., Nizhny Novgorod 603022, Russian Federation

Abstract

Silicon compounds have a wide range of electrical properties. In particular, the possibility of creating thermoelectric converters based on them looks extremely attractive. The use of most silicides as thermoelectrics today is limited by their low efficiency. The development of approaches consisting in the creation of low-dimensional structures using non-equilibrium formation methods is one of the priority directions for improving the properties of thermoelectric generators. Determination of the effect of technological regimes on the structure, phase-chemical composition and thermoelectric properties of metal-silicide structures is a key task, the solution of which will allow creating highly efficient thermoelectric generators based on them.

Thin-film structures with a layer thickness of ~50 nm formed at different growth temperatures by pulsed laser deposition on two types of substrates: sapphire and gallium arsenide coated with an Al_2O_3 nanolayer were studied in this work. On the formed samples, a chemical analysis and a study of the phase composition were performed. Chemical analysis was carried out by X-ray photoelectron spectroscopy with the chemical composition depth profiling. The phase composition was studied by Raman spectroscopy. In addition, analysis of the elements in the films was carried out by X-ray spectral microanalysis based on a scanning electron microscope. To determine the thermoelectric properties of the formed thin-film structures, the temperature dependences of the Seebeck coefficient and the electrical conductivity coefficient were recorded.

The dependence of the thermoelectric characteristics of iron silicide films on the phase composition is analyzed. In particular, measurements of the thermoelectric properties of FeSi_x thin-film structures registered the manifestation of a strong thermoelectric effect in layers with the maximum number of chemical bonds between iron and silicon. The parameters of the growth process at which the most effective formation of iron-silicon chemical bonds is achieved were determined using the method of X-ray photoelectron spectroscopy. Line shifts from the beta phase of iron disilicide were found in the Raman spectra and the reasons for their appearance were proposed.

Keywords: Iron silicide, Thermoelectric, Pulsed laser deposition, Composition, X-ray photoelectron spectroscopy, Raman spectroscopy *Funding*: The work was carried out within the framework of the project N-487-99 under the program of strategic academic leadership «Priority-2030».

For citation: Nikolichev D. E., Kriukov R. N., Nezhdanov A. V., Zdoroveyshchev A. V., Kuznetsov Yu. M., Lesnikov V. P., Zdoroveyshchev D. A., Dorokhin M. V., Demina P. B., Skrylev A. A. Composition and thermoelectric properties of structures based on iron silicide grown by pulse laser deposition. *Condensed Matter and Interphases*. 20223;25(3): 383–391. https://doi.org/10.17308/kcmf.2023.25/11262

Research article

https://doi.org/10.17308/kcmf.2023.25/11263

Features of the resistive response to ozone of semiconductor PdO sensors operating in thermomodulation mode S. V. Ryabtsev¹, N. Yu. Obvintseva², V. V. Chistyakov³, A. A. K. Al-Habeeb¹, A. V. Shaposhnik⁴, S. Yu. Turishchev¹,

E. P. Domashevskaya¹

¹Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

²University of Science and Technology «MISIS»,

4 Leninskiy pr., Moscow 119049, Russian Federation

³Ioffe Institute,

26 Polytekhnicheskaya st., St. Petersburg 194021, Russian Federation

⁴Voronezh State Agrarian University named after Peter the Great

1 Michurin st., Voronezh 394087, Russian Federation

Abstract

This work is dedicated to the issue of increasing the selectivity of semiconductor PdO sensors in case of ozone detection.

Thin PdO films were obtained using thermal sputtering of Pd and its subsequent oxidation. We characterised the obtained material using X-ray diffraction analysis and optical spectroscopy. We studied the gas-sensing properties of thin films in the mode of periodically changing temperature. The use of the thermal modulation mode allowed discovering the extremes of the resistive response of the PdO sensor in ozone, which helped to increase the selectivity of the sensor while detecting this gas.

We suggested a possible mechanism of ozone chemisorption, which determined the specific form of the thermally modulated PdO response. The studies of the resistive response of PdO sensors under the conditions of ultraviolet illumination confirmed the suggested mechanism of ozone chemisorption.

Keywords: Semiconductor gas sensors, Palladium oxide, Ozone, Thermal modulation mode, Features of resistive response of sensors, Oxygen chemisorption mechanism, Oxygen chemisorption under the conditions of UV illumination

Funding: The study was supported by the Russian Foundation for Basic Research, grant No. 20-03-00901; the Ministry of Education and Science of the Russian Federation in the framework of the state order to higher education institutions in the sphere of scientific research for years 2020–2022, project No. FZGU-2020-0036; the Ministry of Education and Science of the Russian Federation, agreement No. 075-15-2021-1351, regarding automation of electrophysical measurements.

For citation: Ryabtsev S. V., Obvintseva N. Yu., Chistyakov V. V., Al-Habeeb A. A. K., Shaposhnik A. V., Turishchev S. Yu., Domashevskaya E. P. Features of the resistive response to ozone of semiconductor PdO sensors operating in thermomodulation mode. *Condensed Matter and Interphases*. 2023;25(3): 392–397. https://doi.org/10.17308/kcmf.2023.25/11263

Research article

https://doi.org/10.17308/kcmf.2023.25/11264

Features of the molecular composition of dental biofilm in patients depending on the degree of caries and the method of its prevention: synchrotron FTIR spectroscopic studies

P. V. Seredin¹, D. L. Goloschapov¹, V. M. Kashkarov¹, N. S. Builov¹, Yu. A. Ippolitov², I. Yu. Ippolitov², J. Vongsvivut³

¹Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

²Voronezh State Medical University,

10 Studentcheskaya st., Voronezh 394036, Russian Federation

³Australian Synchrotron (Synchrotron Light Source Australia Pty LTD),

800 Blackburn Road, Clayton, Victoria 3168, Australia

Abstract

The article studies the molecular composition of dental biofilm in healthy people and patients with multiple caries lesions during several stages of exogenous and endogenous preventive measures.

The observed changes in the IR spectra registered during different stages of the experiment indicate a lack of balance between demineralisation and mineralisation of hard tissues resulting from different absorption mechanisms of agents applied exogenously and endogenously. All the observed changes result from the difference in the microbiota in healthy patients and patients with caries, as well as the difference in the microbiota caused by the impact of preventive agents on biofilm.

Keywords: Biofilm, Molecular properties, Endogenous and exogenous preventive methods, IR microspectroscopy, Synchrotron radiation *Funding:* This study was supported by Russian Science Foundation, grant No. 23-15-00060.

Acknowledgements: Access to scientific equipment and methodology was provided by the Ministry of Education and Science of the Russian Federation, agreement No. 075-15-2021-1351.

The IRM studies were conducted by means of ANSTO's Australian Synchrotron.

For citation: Seredin P. V., Goloshchapov D. L., Kashkarov V. M., Buylov N. S., Ippolitov Yu. A., Ippolitov I. Yu., Vongsvivut J. Features of the molecular composition of dental biofilm in patients depending on the degree of caries and the method of its prevention: synchrotron FTIR spectroscopic studies. *Condensed Matter and Interphases*. 2023;23(3): 398–405. https://doi.org/10.17308/kcmf.2023.25/11264

Research article

https://doi.org/10.17308/kcmf.2023.25/11265

Heat capacities and thermal expansion coefficients of iron triad metals

S. V. Terekhov

Galkin Donetsk Institute for Physics and Engineering

72 R. Luxembourg st., Donetsk 83114, Russian Federation

Abstract

One of the complex problems relating to the thermodynamics of a substance is creating an adequate description of its thermal properties. For example, the Einstein and Debye models (as well as in various modifications of these models) the heat capacity is calculated only when mechanical vibrations of the lattice are taken into account. This leads to the impossibility of describing the increase in heat capacity with increasing temperature for most substances, including iron triad metals. In addition, there is not a single theoretical construction capable of calculating the temperature dependences of the heat capacity and thermal expansion coefficient during polymorphic transformations and structural, magnetic and other phase transitions in the system. They appear on the charts in the form of final jumps, peaks and holes. As a result, there is a need to develop a new approach to the calculation of thermal characteristics. It should take into account the occurrence of local equilibrium in small areas in initially non-equilibrium metal samples for research. The nonequilibrium of a sample can be caused by the presence of impurity atoms, defects, volatile components in it, residual stresses, the occurrence of irreversible processes, etc. For the analytical description of arrays of measured values, experimenters use different exponential expressions in different temperature intervals, sometimes with negative powers. Such theoretical and experimental approaches cannot be considered satisfactory. Therefore, for the creation of the new model, it is necessary to choose such values that would be sensitive to changes in the state of the system. Within the framework of the proposed model of a two-phase locally equilibrium region, such quantities are the absolute temperature of the system, the order parameter in the form of the difference in volume fractions of coexisting ideal phases, the phase composition of the ordering phase, and its derivative with respect to temperature. The developed model allows to calculate the temperature dependences of the heat capacities and coefficients of thermal linear expansion of the iron triad metals (Fe, Co, Ni) with a change in the aggregation state (crystal - liquid), the presence of structural, magnetic and other phase transitions.

It has been shown that the used expressions adequately describe the experimental data in a wide temperature range, and also allow to extend the plotted curves to experimentally unexplored regions. A possible structural transition in cobalt at a temperature of about 1600 K, the existence of which requires additional experiments, was established. The obtained expressions are distinguished by their simplicity and universality of applicability; they can be used to create an automatic calculation of the thermophysical properties of not only iron triad metals, but also other solid substances.

Keywords: Thermodynamic model, Order parameter, Structural rearrangement, Polymorphic transformations, Transition metal *For citation:* Terekhov S. V. Heat capacities and thermal expansion coefficients of iron triad metals. *Condensed Matter and Interphases*. 2023;25(1): 406–414. https://doi.org/10.17308/kcmf.2023.25/11265

Research article

https://doi.org/10.17308/kcmf.2023.25/11266

Temperature influences of the interfacial layer in MOS (Pt/TiO₂/Si) structures

H. D. Chandrashekara, P. Poornima

Government science college (Autonomous), Department of Physics,

Hassan 573201, Karnataka, India

Abstract

In this paper present *I*-*V* and *C*-*V* electrical characteristics of MOS (Pt/TiO₂/Si) were reported. In the *I*-*V* characteristics the various electric parameter estimated such as the ideality factor (*n*), barrier height (Φ_B), leakage current (I_c) and saturation current (I_o) were estimated and further analyzed with Cheung functions.

These electrical parameters were observed to be varying with heat treatment. The *C-V* characteristics, flat band voltage $(V_{\rm FB})$, interface trap density $(D_{\rm it})$, effective charge density $(N_{\rm eff})$ and oxide trapped charge $(Q_{\rm ot})$ were estimated and analyzed. The variation of these values with annealing temperature was correlated with restructuring and rearrangement of TiO₂/SiO₂ atoms at the metal/silicon interface. The hysteresis loop in counter clock wise voltage between -1 V to 1 V at 1 MHz frequency, after 600 °C heat treatment show the strong accumulation region, this may be due to the reduced interface trapped charge and dangling bond.

Keywords: Leakage current, Ideality factor, Flat band voltage, Oxide trapped charge

Acknowledgement: Authors would like to thank Indian Nano electronics User's Programme, Centre for Nano Science and Engineering (CeNSE). One of the author (HDC) thank all the staff of GSC, Hassan, for their moral support to do the research work.

For citation: Chandrashekara H. D., Poornima P. Temperature influences of the interfacial layer in MOS (Pt/TiO₂/Si) structures. *Condensed Matter and Interphases*. 20223;25(3): 415–423. https://doi.org/10.17308/kcmf.2023.25/11266

Research article

https://doi.org/10.17308/kcmf.2023.25/11391

Sedimentation of bentonite suspensions under the influence of low molecular weight polymers based on amino ester salts

D. Yu. Vandyshev¹, **O. V. Sleptsova¹**, **V. Yu. Gazin¹**, **S. A. Malyutin²**, **N. R. Malkin²**, **Kh. S. Shikhaliev¹ Voronezh State University,**

1 Universitetskaya pl., Voronezh 394018, Russian Federation

²JSC Petrochem,

14, Rabochaya st., Belgorod 308017, Russian Federation

Abstract

Among the available technologies for treating natural and wastewater from clay materials, coagulation/flocculation is the most common method due to its high efficiency, simplicity, and cost-effectiveness. Inorganic coagulants such as aluminum sulfate and ferric chloride, widely used as destabilizing agents for colloidal particles, have several significant drawbacks: low efficiency and toxicity. Organic reagents of both natural and synthetic origin are a good alternative.

This work is devoted to the evaluation of the flocculation action of new reagents, which are low molecular weight polymers based on amino ester salts on clay suspensions, as well as the selection of their optimal concentration, providing the maximum sedimentation rate.

Studies have shown that amino ester salts can be effectively used for the treatment of water-clay suspensions. An important factor is the nature of the anion used, which has a significant influence on the coagulation ability of esters. Thus, 40-50 % (wt.) aqueous solutions of amino ester chlorides added to clay suspensions in an amount not exceeding 0.1% (vol.) can be used to thicken clay suspensions. At the same time, aqueous solutions of amino ester bromides regardless of the concentration, introduced into bentonite suspensions of 0.1-0.4 % (vol.), contribute to improved sedimentation, reducing viscosity, and increasing filtration capacity. These results allow us to recommend the use of amino ester chlorides as a thickener in the preparation of drilling muds for strengthening the walls of wells during drilling, and bromides – for flocculation of bentonite suspensions in oil production.

Keywords: Flocculation, Coagulation, Amino esters, Sedimentation rate, Rheological properties, Bentonite, Drilling fluid

Funding source: The results were obtained as part of the work supported by the Ministry of Science and Higher Education of the Russian Federation within the framework of the state assignment to universities in the field of scientific activity for 2022-2024, project No. FZGU-2022-0003.

Acknowledgments: Research results were partially obtained on the equipment of the Collective Use Centre of Voronezh State University. URL: http://ckp.vsu.ru

For citation: Vandyshev D. Yu., Sleptsova O. V., Gazin V. Yu., Malyutin S. A., Malkin N. R., Shikhaliev Kh. S. Sedimentation of bentonite suspensions under the influence of low molecular weight polymers based on aminoether salts. *Condensed Matter and Interphases*. 20223;25(3): 424–434. https://doi.org/10.17308/kcmf.2023.25/11391

Research article

https://doi.org/10.17308/kcmf.2023.25/11393

Inhibitors of chloride corrosion of reinforcement steel

in concrete based on derivatives of salts of carboxylic acids and dimethylaminopropylamine

O. A. Kozaderov, D. S. Shevtsov, M. A. Potapov, I. D. Zartsyn, S. N. Grushevskaya, A. A. Kruzhilin, E. A. Ilina, K. A. Tkachenko, Kh. S. Shikhaliev

Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

Abstract

In our study, we synthesised derivatives of salts of carboxylic acids and dimethylaminopropylamine: 3-(dimethylamino)propyl-1-ammonium acetate, 3-(dimethylamino)propyl-1-ammonium hexanoate, 3-(dimethylamino)propyl-1-ammonium octanoate, and 3-(dimethylamino)

propyl-1-ammonium terephthalate. The structures of the molecules of the obtained substances were confirmed using physical methods: Fourier-transform infrared spectroscopy, NMR spectroscopy, and HPLC.

Electrochemical methods (voltammetry and electrochemical impedance spectroscopy) and quantum chemical modeling were used to assess the inhibitory effect of the synthesised substances with regard to 35GS reinforcement steel. Experiments were conducted in a water extract from a mortar simulating concrete pore solution in the presence of chlorides inducing pitting corrosion. 3-(dimethylamino)propyl-1-ammonium terephthalate is expected to have the highest degree of protection (up to 71%) at a concentration of 2.0 g·dm⁻³. The highest degree of protection for the derivatives with alkyl radicals is 41–46% in a range of concentrations from 0.5 to 2.0 g·dm⁻³. The results of potentiodynamic measurements and quantum chemical modeling were close. Average level of degree of protection can be explained by a high concentration of chlorides in the model solution (1.00 mol·dm⁻³). The effectiveness of the obtained substances is to be further studied using fine-grained concrete. This will help to assess the impact of the additives on the capillary pore structure (permeability) of concrete and the concentration of chlorides.

Keywords: Reinforcement steel, Reinforced concrete, Corrosion inhibitors, Chlorides, Dimethylaminopropylamine derivatives *Funding:* The study was supported by the Russian Science Foundation (RSF), project No. 22-23-01144, https://rscf.ru/en/project/22-23-01144/ *For citation:* Kozaderov O. A., Shevtsov D. S., Potapov M. A., Zartsyn I. D., Grushevskaya S. N., Kruzhilin A. A., Ilina E. A., Tkachenko K. A., Shikhaliev Kh. S. Inhibitors of chloride corrosion of reinforcement steel in concrete based on derivatives of salts of carboxylic acids and dimethylaminopropylamine. *Condensed Matter and Interphases*. 2023;25(3): 435–444 . https://doi.org/10.17308/kcmf.2023.25/11393

Research article

https://doi.org/10.17308/kcmf.2023.25/11396

Evaluation of the inhibitory effect of some derivatives of salts of long-chain carboxylic acids in relation to pitting corrosion of reinforcing steel in concrete

O. A. Kozaderov, D. S. Shevtsov, M. A. Potapov, I. D. Zartsyn, S. N. Grushevskaya, A. A. Kruzhilin, E. A. Ilina, K. A. Tkachenko, Kh. S. Shikhaliev

Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

Abstract

Derivatives of salts of long chain carboxylic acids and dimethylaminopropylamine, including those similar in composition to vegetable oils were synthesized. The structure of the molecules of new substances was reliably confirmed using physical methods of IR-Fourier spectroscopy, NMR spectroscopy, and HPLC.

The inhibitory effect of the synthesized substances on 35GS grade reinforcing steel was assessed using voltammetry. Experiments were carried out in an aqueous extract from a mortar, simulating the concrete pore solution, in the presence of chlorides as activators of pitting corrosion, as well as in samples of fine-grained concrete with periodic immersion in a chloride solution. It was found that 3-(dimethylamino) propyl-1-ammonium stearate did not exhibit an inhibitory effect. The introduction of salts of fatty acids of coconut and sunflower oils increased the anti-corrosion properties. The degree of protection was 40-44% in aqueous solutions and 30-32% for concrete samples. The time before the onset of corrosion in concrete samples was found to increase by 1.75 times compared to the control composition without additives.

Keywords: Reinforcing steel, Reinforced concrete, Corrosion inhibitors, Chlorides, Long-chain salts carboxylic acids

Funding: The study was supported by the Russian Science Foundation (RSF), project no. 22-23-01144, https://rscf.ru/en/project/22-23-01144/ *For citation:* Kozaderov O. A., Shevtsov D. S., Potapov M. A., Zartsyn, I. D., Grushevskaya S. N., Kruzhilin A. A., Ilina E. A., Tkachenko K. A., Shikhaliev Kh. S. Evaluation of the inhibitory effect of some derivatives of salts of long-chain carboxylic acids in relation to pitting corrosion of reinforcing steel in concrete. *Condensed Matter and Interphases*. 2023;25(3): 445–453. https://doi.org/10.17308/kcmf.2023.25/11393

Research article

https://doi.org/10.17308/kcmf.2023.25/11398

Localization of the E. coli Dps protein molecules in a silicon wires under removal of residual salt

E. V. Parinova¹, S. S. Antipov⁷, V. Sivakov³, E. A. Belikov¹, O. A. Chuvenkova¹, I. S. Kakuliia¹, S. Yu. Trebunskikh¹, K. A. Fateev¹, M. S. Skorobogatov¹, R. G. Chumakov¹, A. M. Lebedev⁴, O. V. Putintseva¹, V. G. Artyukhov¹, S. Yu. Turishchev¹

¹Voronezh State University,

1 Universitetskaya pl., Voronezh 394018, Russian Federation

²Institute of Cell Biophysics of the Russian Academy of Sciences,

3 Institutskaya ul., Pushchino 142290, Russian Federation

³Leibniz Institute of Photonic Technology, Department Functional Interfaces,

Albert Einstein Str. 9, 07745 Jena, Germany

⁴National Research Center "Kurchatov Institute",

1 Akademika Kurchatova pl., Moscow 123182, Russian Federation

Abstract

The work is related to the removal of residual salts in hybrid structures formed as a result of silicon wires arrays combining with a nanomaterial of natural origin – bacterial ferritin-like protein Dps. The study of the morphology and composition of the surface and the bulk part of the hybrid structure as a result of combination and subsequent washing in water was carried out.

The method of metal-assisted wet chemical etching was used to obtain silicon wires arrays. To obtain recombinant protein, *Escherichia coli* BL21*(DE3) cells with chromatographic purification were used as producers. The combination of silicon wires with protein molecules was carried out by layering them in laboratory conditions, followed by drying. The residual salt found earlier in the hybrid material was removed by washing in water. The resulting hybrid material was studied by scanning electron microscopy and X-ray photoelectron spectroscopy. A well-proven complementary combination of scanning electron microscopy and X-ray photoelectron spectroscopy together with ion etching was used to study the morphology of the hybrid material "silicon wires – bacterial protein Dps" and the composition with physico-chemical state respectively.

In arrays of silicon wires with a wire diameter of about 100 nm and a distance between them from submicron to nanometer sizes, protein was found as a result of layering and after treatment in water. At the same time, the amount of residual NaCl salt is minimized on the surface of the hybrid structure and in its volume.

The obtained data can be used in the development of coating technology for the silicon wires developed surface available for functionalization with controlled delivery of biohybrid material.

Keywords: Nanostructures, Biomolecules, Hybrid materials, Developed surface, Recombinant ferritin-like protein Dps, Silicon wires, Scanning Electron Microscopy, X-ray Photoelectron Spectroscopy

Funding: The study was supported by Russian Science Foundation (Project 19-72-20180). The work is supported under scholarship of the President of Russian Federation SP-189.2021.1 for young scientists in part of the silicon wires arrays formation, the methodology of work with protein molecules from E.coli cell material. V.S. gratefully acknowledges financial support by the German Research Foundation (DFG) under Grant SI 1893/18-1.

For citation: Parinova E. V., Antipov S. S., Sivakov V., Belikov E. A., Chuvenkova O. A., Kakuliia I. S., Trebunskikh S. Yu., Fateev K. A., Skorobogatov M. S., Chumakov R. G., Lebedev A. M., Putintseva O. V., Artyukhov V. G., Turishchev S. Yu, Localization of the E.coli Dps protein molecules in a silicon wires under removal of residual salt. Condensed Matter and Interphases. 2023; 25(3): 454-461. https://doi. org/10.17308/kcmf.2023.25/11398

Short communications

Research article

https://doi.org/10.17308/kcmf.2023.25/11268

Mass spectrometry of complex compound of bis-thiourea-lead (II) chloride M. Yu. Krysin¹, V. N. Semenov¹, T. V. Samofalova¹, N. M. Ovechkina² ¹Voronezh State University, 1 Universitetskaya pl., Voronezh 394018, Russian Federation

²Voronezh State Medical University named after N. N. Burdenko, 10 Studencheskaya st., Voronezh 394036, Russian Federation

Abstract

Complex compounds of lead salts and thiourea are of interest due to the possibility of their practical application as precursors in the deposition of metal sulphide films. It is relevant to establish the relationship between the composition and structure of the initial complex compounds and the structure of the sulphides formed as a result of their thermal destruction. This paper presents the results of studying the complex compounds formed in an aqueous solution of lead chloride and thiourea.

The structure of the complex compounds was determined by matrix-assisted laser desorption/ionisation mass spectrometry. The mass spectrometry data confirmed the formation of the [Pb((NH₂)₂CS)₂Cl₂] complex in the solution, which is a precursor in the deposition of PbS films. It was demonstrated that mass spectrometry fragmentation of the molecular ion of the [Pb((NH₂)₂CS)₂Cl₂] compound leads to the formation of a lead sulphide ion.

The obtained data confirm the formation of the lead-sulphur bonds in the inner sphere of the complex compound, which are fragments of the crystal structure of the prospective sulphide formed during the thermolysis of the complex.

Keywords: thiourea complex compounds, complexation, lead sulphide, mass spectrometry

For citation: Krysin M. Yu., Semenov V. N., Samofalova T. V., Ovechkina N. M. Mass spectrometry of complex compound of dichlorodithiocarbamide lead (II). Condensed Matter and Interphases. 2023;25(3): 462-466. https://doi.org/10.17308/kcmf.2023.25/11268