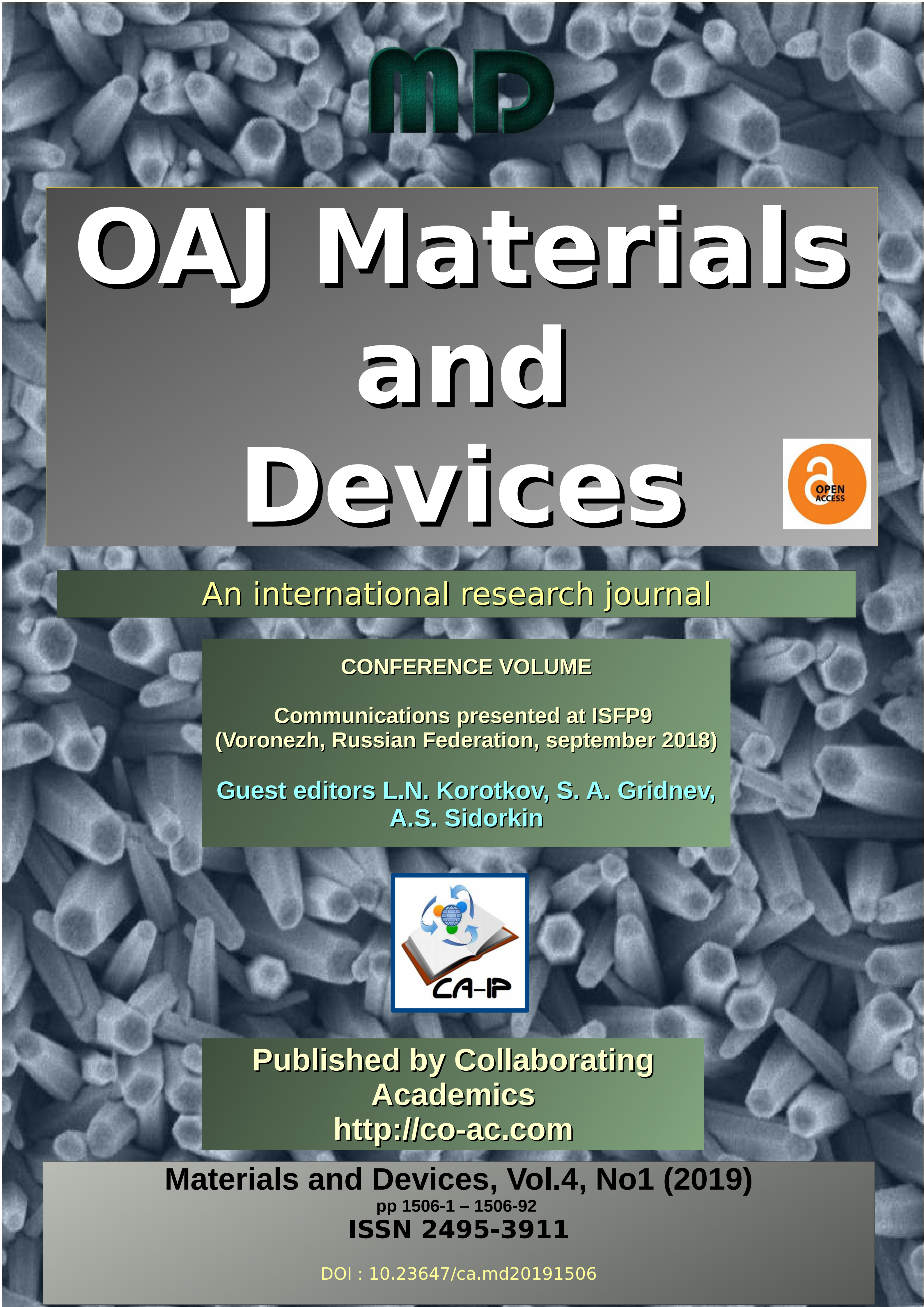

OAJ Materials and Devices

An international research journal

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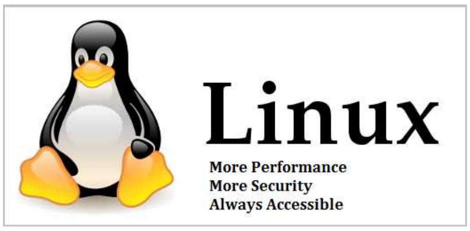

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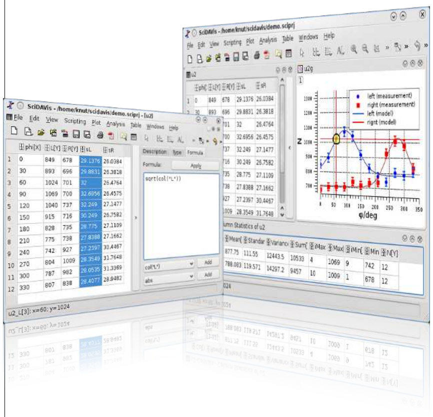

ABSTRACTS BOOK

The Ninth International Seminar on Ferroelastic Physics

Organized by
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The Russian Academy of Sciences
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2018

Voronezh, RUSSIA

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THE PHYSICS OF FERROELASTICS CONTINUES TO EVOLVE

S.A Gridnev and L.N. Korotkov

Ferroelastics are the crystals having spontaneous deformation of the crystal lattice in a certain temperature range, which can be reoriented by external mechanical stress.

The term “ferroelastics” was firstly introduced by Aizu at 1969 year [1]. Somewhat later, Aizu proposed the concept of higher order ferroics [2], which allowed him to construct a unified phenomenological systematics of crystals undergoing structural phase transitions with a change in symmetry point group. These are ferroelectrics, ferroelastics, ferromagnetics and ferroics of higher orders. The phase transitions and the anomalies of the physical properties accompanying them in all these types of crystals are described in terms of the Landau theory and have many common features accordingly. However, at the same time they have fundamental differences.

Feerroelastics are characterized by softening of acoustic modes in the case of proper phase transitions, the specific nature of the fluctuations of the order parameter and by specific effect of defects on the lattice dynamics near the phase transition point. Moreover, they are characterized by the special nature of the anomalies of elastic and piezooptic properties, by specific dynamics of domains, which are themselves specific, etc.

Ferroelastics are the most numerous class of crystals, undergoing structural phase transitions, and at the same time, the most convenient objects for their study. Besides, ferroelastics begin to be used more and more in the new technique. For these reasons, interest in them continues to grow, as clearly demonstrated by the regularly held seminars on the Ferroelastics Physics. (The foregoing is taken from [3])

The regular 9(14) International Seminar on Ferroelastic Physics (ISFP - 9(14)) was organized at September 2018 by the Laboratory of Ferroelectrics of the Voronezh State Technical University in collaboration with the Scientific Council on Ferroelectrics and Dielectrics of the Russian Academy of Sciences and the Ministry of Education of Russian Federation. It was the fourteenth event in a series that began at Bologoe, Russia, in 1978 and was initiated by Prof. L.A. Shuvalov for the purpose of conveying a better understanding of ferroelastic properties in crystals undergoing different structural phase transitions. This and subsequent seminars (Voronezh – 1982, Kharkov – 1985, Dniepropetrovsk – 1988, Uzhgorod – 1991, Voronezh – 1994, Kazan – 1997, Voronezh – 2000, 2003, 2006, 2009, 2012, 2015) provided the panel for the scientific discussions on all the important aspects of the ferroelasticity.

The ISFP - 9(14) was held on the eve of the 50th anniversary of the publication of the first work devoted to ferroelastics. The seminar has demonstrated, that the physics of ferroelastics, despite of all difficulties, prolongs is developed successfully.

Traditionally, a large number of works presented in ISFP-9(14) are devoted to lattice dynamics and structural phase transitions in various classes of ferroics and multiferroics. Judging by the contributions presented, in interpreting the experimental results, the methods of the phenomenological theory were used more often than others.

A considerable number of experimental and theoretical works sent to study of the physical properties of weakly ordered ferroics and various heterogeneous materials with a micro- and nano-scale inhomogeneities, including superlattices of the ferroelectric – ferroelectric or ferroelectric – dielectric type. Of particular interest to such structures is associated with their unusual physical properties. Among the heterogeneous materials discussed in the course of the seminar, one should also single out structures of the ferroelectric-ferromagnet type.

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I. Plenary Lectures

Thermodynamic Method in the Study of Phase Transitions and Caloric Effects in Ferroics

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The active and comprehensive application of the thermodynamic method of research in various areas of solid-state physics is largely due to its universality. Indeed, the thermodynamic properties being related to the energy functions certainly respond with their change to any processes occurring in the systems when internal and external parameters are changed – chemical composition, temperature, pressure (uniaxial or hydrostatic), electric and magnetic fields.

The universality of the thermodynamic approach plays a particularly important role in the study of phase transitions and also the accompanying phenomena and effects in solids since the thermodynamic properties are strongly associated with the order parameters. As a result, this method allows one to obtain rich information about the transformations of the different physical origin: ferroelastic, ferroelectric, ferromagnetic and multiferroic. Moreover, the data obtained using this approach are very useful, first, in constructing and correcting models of structural distortions during displacive and/or order-disorder phase transitions, second, for searching and designing ferroic materials promising for use as effective solid state refrigerants.

In this paper, we present a number of results obtained at the Institute of Physics SB RAS in the study of phase transitions in ferroic and multiferroic materials: crystals, ceramics, composites. The approach used is based on methods that allow obtaining information on heat capacity, entropy, thermal expansion, temperature-pressure and temperature-composition phase diagrams and elasto-, electro- and magnetocaloric effects.

Acknowledgment. The reported study was funded by Russian Foundation for Basic Research, Government of Krasnoyarsk Territory, Krasnoyarsk Regional Fund of Science to the research project № 17-42-2476 “An integrated approach to searching and development of the promising solid ferroic coolants based on single- and multi-caloric effects”

The Application of the THz-IR Spectroscopy for Investigations Dielectric Response Function of a Condensed Matter

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The dielectric response function is one of the most important characteristics that reflect the dynamics of charges in solids. In the THz-IR region, the dielectric response is formed by relaxations and resonance mechanisms that are sensitive to the morphological and structural characteristics of solids. This made THz-IR spectroscopy a convenient method for studying the electro- and magnetodipole characteristics of solids and their parameters that has dependencies on changes in thermodynamic characteristics, morphology, and stoichiometry and impurity concentration. We have used the effectiveness of THz-IR spectroscopy methods for studying both applied and fundamental aspects for a wide class of condensed media such as single crystals, ceramics, glasses and thin films. On the example of ferroelectric ceramics, the peculiarities of the applications of typical methods and approaches to the analysis of experimental data are discussed (fig 1). In this work, the results of investigation of difference absorption processes in dielectric crystals, soft modes in ferroelectrics, the wide band dielectric response of relaxor ceramics, and the feature of absorption in the thin dielectric films are considered. Data on the study of temperature evolution of the dielectric response of organic crystalline compounds are presented.

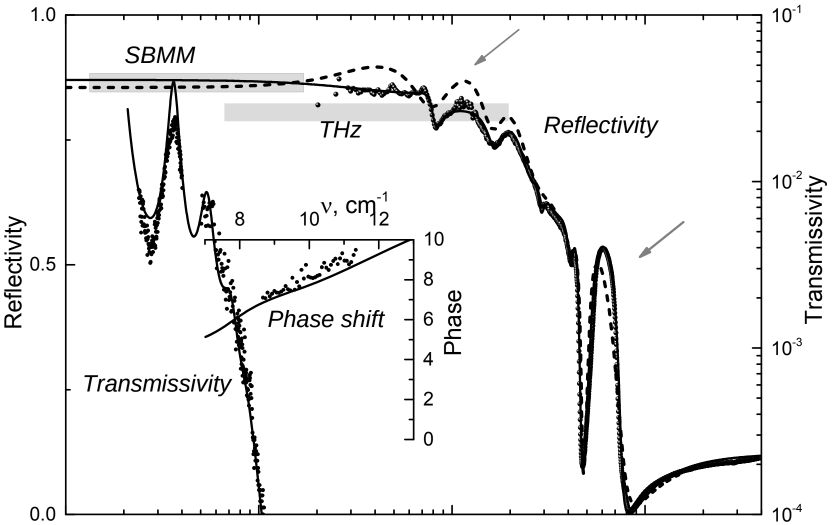

Figure 1. Experimental data analysis including transmissivity, reflectivity and phase shift using the dispersion model of classical oscillator and factorized LST relations [1].

Acknowledgment. This work was supported by Russian Foundation for Basic Research (Grant N 16 -02-00223)

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Brillouin Light Scattering at Structure Phase Transitions in Ferroelectrics and Related Compounds

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In this report, a series of experimental studies of the acoustic response of crystals is considered. It was shown that the analysis of the acoustic response of a crystal must take into account dispersion and fluctuation effects, processes of interaction between relaxation modes, soft modes, and other low-frequency excitations with long-wavelength acoustic phonons. In the talk analyzes the results of studies of the acoustic response of three classes of ferroelectric and related compounds as a function of frequency and temperature. It is shown that, for the case of the coupling of the quadratic order parameter with deformation, the behavior of the velocity and damping of acoustic phonons is strongly modified and is not described in the framework of the Landau theory. The variances of the acoustic response, the manifestation of fluctuational contributions to the dynamics of the crystal lattice and, as a consequence, the appearance of new effects are revealed.

The use of a new generation of multipass Fabry-Perot interferometers in the experiment made possible to consider in detail the low-frequency region of the vibrational spectrum of the crystals under study and to detect the relaxation mode in ferroelectric compounds. Investigations of this excitation, analysis of quasi-elastic light scattering made it possible to make full use of the possibilities of broad-band Brillouin spectroscopy and to separate contributions related to various mechanisms. It is shown that taking into account such excitations, their interaction with acoustic phonons, as suggested by VL. Ginzburg, offers a way to describe the macroscopic properties of ferroelectrics (f.e. dispersion of the dielectric response).

Acknowledgment. This work was supported by Russian Foundation for Basic Research (Grant N 18-02-01084)

Study of the Thermal Characteristics of the Solid Materials by the Method of the Dynamic Pyroelectric Effect

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The method for determining of the thermal diffusivity coefficient, based on periodic heating of one surface of the sample, was first proposed by A.J. Angstrem in 1863. This method was modified by S. Lang [1], who proposed to illuminate by sinusoidal modulated heat flux the upper surface of the material under investigation, which is located on the pyroelectric detector. Passing through the test sample, the temperature wave propagates in the detector. The change in polarization caused by the temperature change in the pyroelectric crystal leads to the appearance of a pyroelectric current in the external circuit (fig.1). When a sinusoidal modulated heat flow is used, a phase shift occurs between the pyroelectric current and the temperature wave, and to determine the thermal diffusivity, it is necessary to obtain the frequency dependences of the pyroelectric current. We proposed [2] to determine the thermal diffusivity by the Thermal Square Wave Method at single-frequency (TSWM), When the sample surface is heated by a rectangular modulated heat flux. The measurements are carried out at a single frequency modulation of heat flux, the time dependence of the pyroelectric current is recorded using an analog–digital converter.

Analysis of the shape and magnitude of the pyroelectric response of the ferroelectric lithium tantalate crystal as a function of the values of the thermal conductivity and thermal diffusion coefficients of the material, through which the temperature wave passes, showed that the use of rectangular modulation of the heat flux makes it possible to vary two parameters when calculating, values of thermal conductivity and thermal diffusivity coefficients [3].

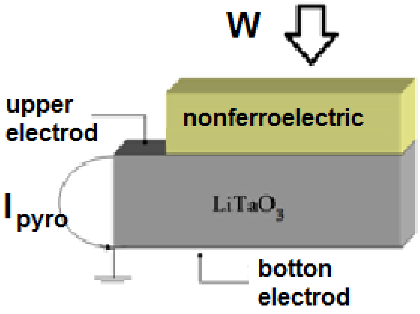

Fig. 1. Scheme for registration of the pyroelectric response when the thermal characteristics are measured by the dynamic method

With the use of mathematical modeling, the shape of the pyro-response is calculated, while the coefficients of thermal conductivity and thermal diffusivity of the sample under study are parameters, which in the calculation is selected in such a way that the calculated form of the pyroelectric response coincides with the experimental one.

Acknowledgment. This work was supported by State Assignment №3.8032.2017/BCh of the Ministry of Science and Education of Russia

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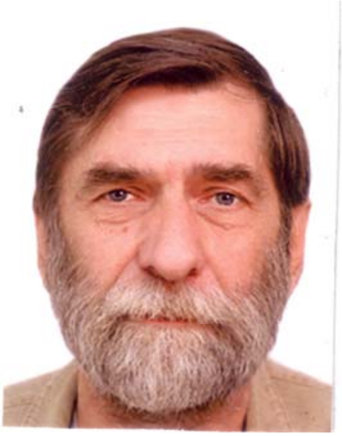
Neutron and X-ray Scatterings for Diagnostics of Ferroelectric and Multifunctional Nanostructures



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This lecture is devoted to application of neutron and X-rays (including synchrotron radiation) scatterings for studies of multifunctional nanostructures prepared on base of various nanoporous media: porous glasses, artificial opals, MCM and SBA structures, chrysotile asbestos. In introduction the short description of morphology and properties of porous matrices is done. The questions and problems related to analysis of diffraction patterns (including determination particles sizes and their forms, appearance of strains, additional information from background analysis, texture and so on) are discussed in the first part. The presented material is illustrated by some examples for ferroelectric and magnetic nanocomposite substances. The second part is devoted to application of small angle neutron (SANS) for attestation porous media and nanocomposites. The advantage of SANS method consists precisely in the fact that it provides an opportunity to obtain information about the spatial organization of the studied samples, including sizes of the particles and their fractal characteristics. In the last part the questions related to experimental studies of atomic dynamics of nanostructured metals by inelastic neutron and synchrotron radiation scattering are considered. The contributions of interface are analyzed for Pb and Sn nanoparticles.

Construction and classification of phenomenological models of phase transitions by the catastrophe theory methods

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The phenomenological theory of phase transitions (PT) must be completely based on rigorous mathematical methods. Group-theoretical analysis makes it possible, on the basis of knowledge of the group of the high-symmetry phase of the G_0 crystal, to list all the low-symmetry phases into which a phase transition is possible, and for each phase to determine the dimension of the order parameters (OP's). Using the theory of invariants, invariant combinations of the OP components (basic invariants), on which the thermodynamic potential depends, are calculated. To determine the phase diagrams and to find the dependences of physical properties on external influences - temperature, pressure, etc. near the points of the PT, it is necessary to proceed to the model representations. Any physical model is a simplified version of the physical system, preserving its main features. And the main features of the thermodynamic system experiencing the PT are global minimality and structural stability. To ensure the thermodynamic stability of the system, the potential should not allow infinitely large fluctuations of OP's, leading to an infinite gain in energy. This requires that the thermodynamic potential has a global minimum at finite values of the OP. The concept of structural stability for the phenomenology of PT is one of the most important. The fact is that only those results that have sufficient repeatability in the experiment can be included in the category of physical phenomena. Hence, the phenomenological model describing the properties of such a system must be structurally stable. The explicit form of the thermodynamic potential according to the Landau theory is given as a finite segment of the expansion in a power series in invariant combinations of OP. Global minimality is ensured by the fact that the members of higher degrees in the decomposition have even degrees and positive coefficients. The condition of structural stability is always satisfied for only one one-component OP. In the case of multicomponent OP, structural stability is not always possible. The use of catastrophe theory methods makes it possible to build a structurally stable phenomenological model. In this case, the initial data are only knowledge of the basic invariants, and the number of control parameters that depend on external thermodynamic quantities (temperature, pressure, chemical potentials of impurities, etc.). And most importantly, such a formulation of the problem allows the classification of phenomenological models according to the number of control parameters for a given set of basic invariants. The beginning of this classification was laid in [1-5].

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The Effect of Compositional Ordering on Relaxor and Magnetic Properties of Ternary Perovskites

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Ferroelectric ternary perovskite oxides of the $PbB'_{1-m}B''_{m}O_6$ (m=1/3 or 1/2) type, are widely used as components of various functional materials exhibiting giant dielectric, electrostrictive, pyroelectric, and piezoelectric responses. Properties of these oxides, especially of the 1:1 type perovskites (m=1/2) depend crucially on the long-range ordering degree S of *B'* and *B"* cations. While in the highly-ordered state a sharp ferroelectric or antiferroelectric phase transition takes place, in the disordered state a relaxor state is observed, characterized by a diffuse and frequency-dependent maximum of the dielectric permittivity.

Previously, to change the S values a long-time annealing was used. Later Li- doping and variation of the conditions of either the crystal growth or high pressure synthesis were successfully used to change the ordering degree of B-site cations in $PbB^{3+}_{1/2}B^{5+}_{1/2}O_3$ perovskites with B^{3+}=Fe, Sc, Yb; B^{5+}=Nb,Ta,Sb. Recently it was found out that high-energy mechanical activation during mechanochemical synthesis stimulates disordering of B^{3+} and B^{5+} cations in ceramics of some 1:1 type perovskites. In some cases it is possible to vary substantially the S values and correspondingly both the temperature and diffusion of dielectric permittivity maxima in these ceramics by changing the regimes of the mechanochemical synthesis and/or using different starting materials (either oxides or preliminary synthesized $B^{3+}B^{5+}O_4$ precursors). The parameters of the dielectric spectra of the samples exhibiting relaxor-like behaviour also depend on the conditions of the mechanochemical synthesis.

Interestingly, the use of mechanochemical synthesis enables one to modify substantially relaxor properties of ceramics of the disordered perovskites $PbFe^{3+}_{1/2}Ta^{5+}_{1/2}O_3$ and $PbMg_{1/3}Nb_{2/3}O_3$. This effect is believed to be caused by the changes of the degree of the short-range ordering. Such explanation is supported by changes in the magnetic phase transition temperature of $PbFe^{3+}_{1/2}B^{5+}_{1/2}O_3$ perovskites-multiferroics (B^{5+} - Nb, Ta) obtained by mechanochemical synthesis. Such ordering is believed to change the number of the magnetic neighbors around each Fe^{3+} ion.

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Microstructural Features, Electrophysical Properties and Wave Process in Ferroelectriceally Active and Dissipative Media

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The objectives of the present work were:

- establishment of fundamental patterns in the formation of the electrophysical properties of porous piezoceramics and composite ferroelectrics, as well as their changes as a result of external influences;
- systematic study of wave processes in spatially inhomogeneous ferroelectric and dissipative media and development of new methods for ultrasonic fields formation for advanced ultrasonic applications.

Objects of the study were:

- porous ferroelectric ceramics based on PZT, lead titanate, sodium-lithium niobate, lead-potassium niobate, lead metanyobate and magnesium niobate etc.;
- ceramic matrix composites «ceramics/ceramics», «ceramics/crystals»;
- samples of biological tissues, viscoelastic and liquid media.

The choice of the selected objects was determined both by the possibility of practical use, and by the specific physical properties of objects.

As a result of systematic complex studies, the following results were obtained and the following conclusions were drawn [1, 2]:

- the character of the dependences of the elastic, dielectric and piezoelectric properties of porous ferroelectric ceramics on porosity is determined by the microstructural features of the piezoceramic skeleton, defined by fabrication methods;
- in the formation of the extreme electrophysical properties of ceramic matrix composites «ceramic/ceramic» and «ceramic/crystal», along with the influence of the properties and structure of the piezoceramic matrix and filler, the microporosity of the piezoceramic matrix arising during sintering plays a decisive role;
- the elastic dispersion and attenuation in porous ferroelectric piezoceramics and ceramic matrix composites are caused by the scattering of elastic waves on the pores and filler particles and are defined by generalized dispersion relations;
- the main mechanisms determining the processes of SAW propagation in ferroelectric ceramics in the presence of an external electric field are the interaction of SAW with moving carriers of the space charge and domain-orientation processes;
- new methods for the formation of high intensity ultrasound fields, dynamical focusing and harmonic excitation, supersonic generation and resonant amplification of shear elastic waves in dissipative media, as well as focusing ultrasonic transducers designs for advanced medical ultrasonic applications have been developed [3].

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Phenomenological Theory of Phase Diagrams of Ferroelastics

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The detailed research of phase diagrams is carried out for Landau's thermodynamic potentials with $L = 3m$ and $43m$ symmetry group [1-7].

In the case $L = 3m$, all possible types of phase diagrams for the sixth-order expansion of thermodynamic potential in terms of the order parameter components are received. Realization conditions for each type of phase diagrams are established, conditions of the multicritical point splitting are studied, and the equations for calculation of tricritical and triple points coordinates are obtained. Surfaces of order parameter components as functions of thermodynamic potential parameters are designed. Qualitative correspondence of phase diagrams theoretical calculations results and an experimental phase diagram is noted at the example of spinel structural type.

In the case $L = 43m$, phase diagrams of the crystals undergoing phase transitions have been constructed within the phenomenological theory of the second-order phase transitions. The equations of state of all phases induced by symmetry have been received, and the general conditions of their thermodynamic stability have been formulated. For the fourth-order expansion of thermodynamic potential in terms of the order parameter components, exhaustive results have been obtained: equations of phases stability boundaries and all possible types of phase diagrams have been found analytically. For the eighth-order expansion of the potential the variety of phase diagrams has been analyzed using computer calculations. For the first time the possibility of existence of phase diagrams described by this potential and containing one or several triple points, three-phase and four-phase regions is shown. Examples of the crystals undergoing phase transitions with considered symmetry of the order parameter have been given.

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Links Between Domain Structures, Heterophases and Phase Contents in Lead-free Ferroelectric Solid Solutions

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Ferroelectric (FE) solid solutions with the perovskite-type structure are of interest because of the important physical properties, various heterophase states and domain structures [1] in compositions near the morphotropic phase boundary (MPB). These solid solutions are also of interest as materials that are applied in solid-state electronics, piezotechnic, hydroacoustic, and other branches. In the last decades, intensive studies on the FE solid solutions are carried out, and their potential applications are discussed, including some applications instead of the traditional FE solid solutions based on $PbTiO_3$ [2]. In the present report, we give a review of results on the problem of links between the non-180° domain (twin) structures in heterophase regions and phase contents in the $BaTiO_3$-based FE solid solutions with compositions near the MPB [3–6].

Our description of the heterophase regions and phase contents is carried out within the framework of models that take into account various orientations of domains (mechanical twins) in FE phases and stress-relief conditions in heterophase regions. Diagrams are built to show links between volume fractions of specific non-180° domain types and polydomain phases that coexist in $(1-x)(Na_{1/2}Bi_{1/2})TiO_3-xBaTiO_3$, $Ba(Ti_{1-x}Me_x)O_3$ (Me = Ce, Zr, Sn, and Hf), and $(Ba_{1-y}Ca_y)(Ti_{1-x}Zr_x)O_3$ near the MPB at room temperature. In some cases, a coexistence of the FE phases is observed at molar concentrations of individual components less than 5%. Conditions for the complete stress relief are analysed at the specific volume fractions of the non-180° domain types and by taking into account specific changes in the unit-cell parameters and the anisotropy of spontaneous strains in the unit cell, all this for compositions near the MPB. Examples of an incomplete stress relief [5] are considered at a coexistence of the FE phases in $(Ba_{1-y}Ca_y)(Ti_{1-x}Zr_x)O_3$. Evaluated volume fractions of the coexisting phases are in agreement with experimental data [3–6].

Our studies show that the developed crystallographic method [1] can be effectively applied to analyse various domain and heterophase states in FE solid solutions at changes in molar concentrations of components in these solid solutions and at changes in the domain (twin) structures and phase contents in samples. The domain structures and their changes as well as stress-relief conditions in heterophase regions are to be taken into account at a prediction of physical properties of the studied materials.

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Relaxation Model of Hysteresis Phenomena in Ferroelectrics: Direct and Inverse Problem

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It is well known that hysteresis effects in condensed systems including ferroelectrics are due to the existence of metastable. Within the framework of the relaxation model, the form of the hysteresis curves of ferroelectrics is due by the following factors [1, 2].

1. Dependence of the order parameter of a single domain on the strength of the external field (including metastable states).
2. The dependence of the probability of switching a single domain from a metastable state to a stable state on the characteristics of the external alternating electric field.

However, in these papers it was assumed that the domain switching processes occur independently of each other. In order to take into account the mutual influence of domains on their switching, it is necessary to take into account internal fields in ferroelectrics.

In this paper we generalize the simple relaxation model [1, 2] of switching processes in ferroelectrics. A closed equation describing the evolution of polarization in ferroelectrics with account of interactions between domains is derived. The analysis of the qualitative properties of the solution of the resulting equation is performed.

The available experimental data on the shapes of the hysteresis curves of a number of ferroelectrics are analyzed, including the dependence of the hysteresis curves shapes on the parameters of the external control field.

It is shown that the regularities observed in the experiment can be explained in the framework of the generalized model. Therefore, experimental data can be used both to refine the microscopic models of ferroelectrics, and to find the parameters of these models.

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II. Phase transitions, lattice dynamics and soft modes

Raman Scattering at Diffuse Phase Transition in $PbB'_{1/3}B''_{2/3}O_3$ Relaxor Ferroelectrics

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The lattice dynamics of relaxor ferroelectrics is studied very actively, but mainly with the example of the widely known compounds $PbMg_{1/3}Nb_{2/3}O_3$ - PMN, $PbMg_{1/3}Ta_{2/3}O_3$ – PMT, etc. The relaxor ferroelectrics $PbCo_{1/3}Nb_{2/3}O_3$ - PCN and $PbNi_{1/3}Nb_{2/3}O_3$ – PNN are considered to be a close analog of the model relaxor ferroelectric PMN [1-2]. They were first synthesized in the form of a single crystal and ceramics in the middle of the 20th century and were studied very pore. Results studies of the lattice dynamics are practically absent. This motivated us to carry out studies of the behavior of the vibrational spectrum of PCN and PNN using Raman scattering of light and compare the results with the data taken from the Raman scattering studies of PMN and PMT.

The measurements were carried out on single crystals of PCN and PNN grown by the method of spontaneous crystallization from a solution to a melt. The structure and composition were monitored by X-ray diffraction and X-ray fluorescence studies. A plates with a polished plane (100) were prepared for Raman measurements. The orientation of the crystals were carried out by x-ray measurements. In light scattering experiments, a LabRam and T6400 spectrophotometers with an optical polarization microscope were used. Temperature measurements were carried out using the Linkam temperature stage with a stabilization accuracy of ± 0.1 degrees. In the experiments, polarized light scattering spectra were obtained in the temperature range from 78 to 680 K. In the high-temperature region, the Raman spectra of PCN and PNN are similar to those observed in PMN and PMT. The temperature dependences of the frequency, the strength of the oscillator, and the intensities of the optical modes were plotted. An anomalous behavior of low-lying optical phonons is observed in the vicinity of the temperature of diffuse phase transition (T_m). The frequency decreases in the vicinity of T_m, and the intensity and strength of the oscillator exhibit anomalous behavior in this temperature range. Analysis of the low-frequency region of the scattering spectrum made it possible to distinguish quasi-elastic scattering (QELS). The temperature behavior of the half-width and the intensity of the QELS demonstrate anomalous behavior at variation of the temperature. The results of the measurements are analyzed in the framework of modern concepts of physics condensed state.

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Short Range Polar Order in the Impurity-Induced Ferroelectric Phase of Incipient Ferroelectrics

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In [1], we developed a method for calculating the magnitude and temperature dependence of the root-mean-square fluctuations of the polarization (short-range, local polar order) $P_{sh} = \langle P^2{}_{fl}\rangle^{1/2}$ below the ferroelectric transition temperature T_c from temperature changes of the spontaneous polar contribution to the refraction of light. This method is especially relevant for the study of systems with the coexistence of long-range and short-range order below T_c, where these contributions are comparable in magnitude. Such systems include incipient ferroelectrics $SrTiO_3$ and $KTaO_3$ doped with impurities ($Sr_{1-x}Ca_xTiO_3$, $SrTi(^{16}O_{1-x}{}^{18}O_x)_3$, $KTa_{1-x}Nb_xO_3$, etc.) in which impurity concentrations higher than the critical value x_c induce ferroelectric ordering. In these objects, the value of $\langle P^2\rangle^{1/2}$, which includes the long-range and short-range orders, is turned out to be significantly greater than the average value of the spontaneous polarization $P_s = \langle P\rangle$ revealing distinctly existence of developed spatial fluctuations of the order parameter, the behavior of which qualitatively differs from the behavior of classical thermodynamic fluctuations near T_c.

This work presents the results of a study of the short-range and long-range polar order, induced by impurities in single crystals $Sr_{1-x}Ca_xTiO_3$ with $x = 0.014$ (SCT-1.4), $SrTi(^{16}O_{0.03}{}^{18}O_{0.97})_3$ (STO-18) and $KTa_{1-x}Nb_xO_3$ with x = 0.018 (KTN). The temperature dependences of the principal values of the refraction of light (specific optical retardation) in SCT-1.4, STO-18 and KTN were measured. The magnitudes and temperature variations of the polar contributions to the principal values of the refraction of light in them were derived. The temperature dependences of the morphic birefringence in SCT-1.4 and dielectric hysteresis loops in SCT-1.4 and KTN were measured to determine P_s. For the quantitative calculation of the P_{sh} value below T_c from experimental data, we used the method developed by us in [1]. As a result we determined the magnitude and temperature dependence of P_{sh} polarization in SCT-1.4, which appears only because of strong spatial fluctuations ("local" or "short-range" ordering) and leads to the contribution of short-range order to the polar phase below and above T_c and the magnitude and temperature dependence of the long-range order polarization P_s. The magnitudes of P_{sh} and P_s were also evaluated in STO-18 and KTN at low temperatures below T_c. The results allowed us to quantitatively establish the role of short and long order in the formation of the impurity-induced polar phase in incipient ferroelectrics.

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On the Main Factors Determining the Phase Transition Temperature in Nanoscale Ferroelastics

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The physical properties of nanoscale ferroelastic particles have been studied much less, both in terms of theory and experiment, in contrast to ferroelectrics, as well as nanocomposites based on them. In theory, this is usually related to a much more complex mathematical model of the ferroelastics properties. As a result, there are no detailed studies of the influence of various factors on phase transitions in ferroelastic nanoparticles. The purpose of this report is research for the main factors determining the phase transition temperature of a ferroelastic nanoparticle and creation an integral picture of the phase transition in it.

In this paper, we consider a functional element of a nanocomposite structure - the ferroelastic plate of size $l \times l \times h$, $l = 100nm$, .

As it is well known, the second-order phase transition occurs by the mechanism of stability loss, therefore, an eigenvalue problem for partial differential equations is chosen as a suitable mathematical apparatus allowing to study various factors in a unified manner and to minimize the volume of computational procedures. The system of equations describing the state of the ferroelastic plate has the following form [1]:

$$-\kappa\Delta\eta - \lambda\eta = \sigma_{13}\,, \tag{1}$$

$$\Delta\sigma_{13} - \frac{3}{1+\nu}\frac{\partial^2 p}{\partial x \partial z} = -\mu\frac{\partial^2 \eta}{\partial y^2}\,, \tag{2}$$

$$\Delta p = -\frac{2}{3}\mu\frac{1+\nu}{1-\nu}\frac{\partial^2 \eta}{\partial x \partial z}, \tag{3}$$

$$\left(\frac{\partial\eta}{\partial\vec{n}} + \frac{\eta}{\delta}\right)\bigg|_{\Gamma} = 0\,,\ \ \sigma_{13}\big|_{\Gamma_x,\Gamma_z} = 0\,,\ \ \frac{\partial\sigma_{13}}{\partial\vec{n}}\bigg|_{\Gamma_y} = 0\,,\ \ p\big|_{\Gamma_y} = 0\,, \tag{4}$$

where $\eta = u_{13}^{(p)}$ is spontaneous (elastic) shear deformation, which plays the role of the order parameter η in the phase transition as in *KH₃(SeO₃)₂*; σ_{13} is component of elastic stress tensor σ_{ik}, $p = -(\sigma_{11}+\sigma_{22}+\sigma_{33})/3$, κ is correlation constant, δ is extrapolation length, μ is shear modulus, ν is Puasson's factor, $\vec{n}$ is unit vector of the outer normal to the plate surface Γ, $\Gamma = \Gamma_x \cup \Gamma_y \cup \Gamma_z$, Γ_j is plate surface perpendicular to axis j, $j = x, y, z$.

We consider the problem (1) - (4) as the eigenvalue problem with respect to λ. Solving it, we obtain a set of eigenfunctions $\{\eta_n\}$ and eigenvalues $\{\lambda_n\}$. The first eigenvalue λ_0 determines the phase transition temperature of the ferroelastic plate:

$$T_0 = T_C - \frac{\lambda_0}{\alpha_0}, \tag{5}$$

where T_C is Curie temperature of a bulk ferroelastic crystal, α_0 is Landau's coefficient for the quadratic term of the expansion of the free energy of a bulk ferroelastic crystal.

In this paper we studied an influence of thickness plate and the extrapolation length to the phase transition temperature.

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Lattice Dynamics and Phase Transitions in Eplasolite-Like Fluorides – Raman Scattering Study

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Crystals of elpasolite-like fluorites A_2BReF_6 (space group of the high symmetry phase is $Fm3m$, $Z = 4$) belong to a wide family of perovskites studied intensively for decades. Such interest to fluorides is due to numerous phases and phase transitions observed in this family [1] as well as their perspective applications: normally their transparency window is much wider than that of more traditional oxides while their spectral properties may be varied easily by partial or complete substitution of rare earth ions Re^{3+}.

Most of phase transitions in perovskite-like crystals are induced by displacements of a central ion in ReX_6 octahedrons or by rotations of these octahedrons due to soft phonon modes condensations. Such condensations have been found many times in chlorine-, bromine- and oxygen-containing elpasolites (see, a. g., [2–4]), but only occasionally in fluorides [5]. Here we present Raman scattering investigations of lattice dynamics in several fluorides with elpasolite structures.

Samples have been synthesised from melt as described in [5,6] and cut along crystallographic axes of the cubic phase. Raman spectra have been obtained with Jobin Yvon – Horiba T-64000 spectrometer and Ar+ laser (514.5 nm, 50 mW), CCD detection with liquid nitrogen cooling, 600 s accumulation time. To interpret results empirical simulations with LADY software and first principle VASP were performed.

High temperature phase of all studied crystals is cubic, and no indications of lattice disorder were found; observed temperature dependences of phonon dampings correspond to normal anharmonic decay. Cooling down and shortening of interionic distances result in lowering of the low frequency phonon dispersive branch in Γ–X direction and instability of the cubic phase. Eigenvectors of this branch in the cubic phase correspond to rotations of ReX_6 octahedrons, while in the lower temperature monoclinic phase they mix with cations displacements. In crystals with relatively lightweight rare earth ions (Sc, In) temperature dependences of higher frequency phonons correspond to phase transitions of the first order, closer to the second one, while in crystals with heavier ions (Ho, Dy) this intermodal interaction becomes stronger and their cubic phase transforms into the monoclinic one directly by the first order phase transition. In contrast to “classical” soft mode restorations we observed in these crystals strong interactions of main and secondary order parameters fluctuations that reduce the range of the intermediate tetragonal phase for heavier rare earth ions.

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Features of the phase transition in a thin ferroelastic plate

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In the present work, it is shown that in a thin ferroelastic film in a definite thickness range a phase transition take place to a nonuniform «domain-like» state. This behavior of the ferroelastic phase is associated with the competition of various contributions to the film free energy and determined near the phase transition point by the expression

$$F = \frac{1}{V}\int\left[-\frac{\alpha}{2}\eta^2 + \frac{\kappa}{2}\left(\nabla\eta\right)^2 - \sigma_{xz}\eta + \frac{\lambda}{2}u_{ii}^{(e)2} + \mu u_{ij}^{(e)2}\right]dV + \frac{1}{S}\int\limits_S \frac{\alpha_s}{2}\eta^2 dS\,, \tag{1}$$

where $\alpha = \alpha_0\left(T_C - T\right)$ is the coefficient of free energy expansion, proportional deviation temperature T from Curie temperature T_C of infinite crystal; κ is the correlation constant; σ_{xz} is the external stress, conjugated order parameter η; λ, μ are the Lame coefficients; $u_{ij}^{(e)}$ is the elastic deformation tensor; α_s is the parameter, proportional to the magnitude of film planes interaction with medium. Varying the functional (1) we get the linear equation with boundary conditions

$$\kappa\Delta\eta + \alpha\eta + \mu\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} - 2\eta\right) = 0\,; \tag{2}$$

$$\alpha_s\eta \mp \kappa\left.\frac{d\eta}{dz}\right|_{z=0,l} = 0\,, \tag{3}$$

where u_x, u_z are the components of displacement vector, l is the film thickness. The equation (2) is need to solve together with equations of elastic equilibrium [1]

$$\begin{cases} \dfrac{\partial^2 u_x}{\partial x^2} + \dfrac{\partial^2 u_x}{\partial z^2} + \dfrac{1}{1-2\nu}\dfrac{\partial}{\partial x}\left(\dfrac{\partial u_x}{\partial x} + \dfrac{\partial u_z}{\partial z}\right) - 2\dfrac{\partial\eta}{\partial z} = 0, \\ \dfrac{\partial^2 u_z}{\partial x^2} + \dfrac{\partial^2 u_z}{\partial z^2} + \dfrac{1}{1-2\nu}\dfrac{\partial}{\partial z}\left(\dfrac{\partial u_x}{\partial x} + \dfrac{\partial u_z}{\partial z}\right) - 2\dfrac{\partial\eta}{\partial x} = 0, \end{cases} \tag{4}$$

where ν is the Poisson's ratio. In the case of various fixed film planes, which considered (3), we obtain a homogeneous system of linear equations for the integration constants of the functions η, u_x, u_z. Equality zero of its determinant defines the phase transition temperature T_f, depending on the film parameters l, μ, ν, α_s and on wave vector k_x, characterizing nonuniform ferroelastic state. The real phase transition temperature corresponds to the maximum of the function $T_f = f\left(k_x\right)$ with a nonzero value k_x and consistent with the ferroelectric films case [2].

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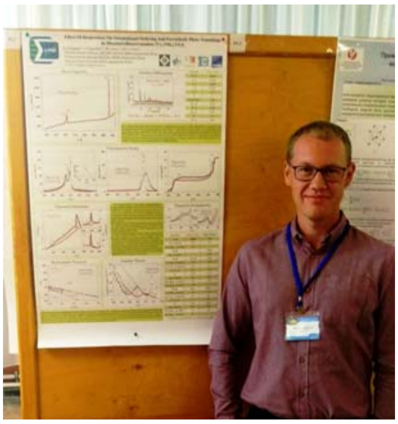
Effect of Deuteration on Orientational Ordering and Ferroelastic Phase Transitions in Dioxotetrafluorovanadate $(NH_4)_3VO_2F_4$



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The crystals of vanadium oxyfluorides (VOF) can form various distorted VOF-octahedra due to the ability of vanadium to adopt different valence. VOF-elements can be used to create crystalline structures with interesting physical properties for designing functional elements in electronics and microelectronics, and can also be considered as materials for creating solid-state cooling devices. Despite the variety of vanadium oxyfluorides, the VOF anion is disordered. In particular, the structure $(NH_4)_3VO_2F_4$ contains two independent OF-anions one of which is orientationally disordered and other is completely ordered [1]. The crystal $(NH_4)_3VO_2F_4$ undergoes four successive phase transitions with with the following symmetry change: $Fm3m \leftrightarrow Immm \leftrightarrow$ rhombic $\leftrightarrow P112/m \leftrightarrow P1$ at T_1=448K, T_2=244K, T_3=210K and T_4=205K respectively.

In the present work, the studies of disordering/ordering processes using deuteration of the ammonium group [2] and complex thermophysical and dielectric studies of crystals $(NH_4)_3VO_2F_4$ have been performed. It was found that deuteration has practically no effect on the temperature of the phase transitions T_1=437K, T_3=212K and T_4=208K but led to the disappearance of the transformation *Immm* ↔ *rhombic* at T_2 (Fig. 1*a*). As a result of D→H substitution, the total entropy change (ΔS_Σ=12.3 J/mol·K → 17.0 J/mol·K) but the contribution from low-temperature transformations has changed insignificantly (Fig. 1*b*). The substitution D→H led to large change in the susceptibility to external hydrostatic pressure the of low-temperature transformations (dT_3/dp=-43 K/GPa → -27 K/GPa and dT_4/dp=-79 K/GPa → -25 K/GPa). The phase *P*112/*m* becomes more stable under pressure in spite of the fact that in $(NH_4)_3VO_2F_4$ it was wedged out at low pressure ($p_{trp} \approx 0.3$ GPa). The nature of the phase transitions remains ferroelastic. Significant changes in the thermal expansion are observed at the high-temperature transformation at T_1 ($\delta\beta_1$=0.6%), that shows the first order of phase transition is preserved.

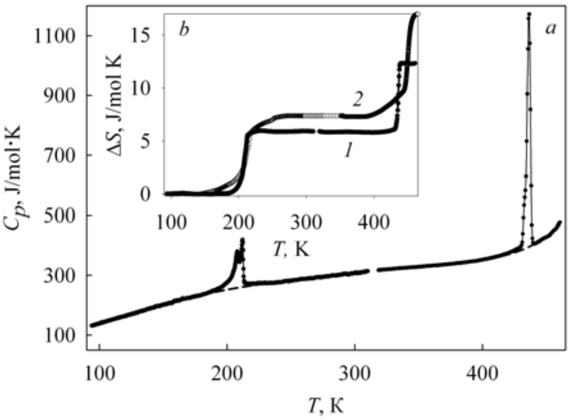

Fig 1. Temperature dependence of the molar heat capacity in a wide temperature range (*a*). Temperature dependence of the total excess entropy change $(ND_4)_3VO_2F_4$ (*1*) and $(NH_4)_3VO_2F_4$ (*2*) (*b*).

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The Effect of Annealing on the Structure and Phase Transitions of $Na_{0.95}Li_{0.05}NbO_3$

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Lead-free $Na_{1-x}Li_xNbO_3$ (NLN) solid solutions are prospective piezoelectronic materials because of a unique combination of parameters, not available in other piezoelectrics. Properties and phase transition temperatures of NLN ceramics depend considerably on the sample's thermodynamic prehistory due to several competing structural instabilities typical of $NaNbO_3$ and its solid solutions [1].

Previously we found out that a long-time (several hours) annealing of NLN ceramics at temperatures below the temperature T_m of the dielectric permittivity ε maximum increases T_m by 20-30 K [2]. However substantial changes of T_m were observed only after annealing in a very narrow temperature range [2,3].

We carried out dielectric, X-ray diffraction and heat capacity studies of the effect of annealing on the properties of $Na_{0.95}Li_{0.05}NbO_3$ (NLN-5) composition. A giant increase of T_m exceeding 60 K was achieved by annealing at different temperatures within a wide temperature range. However the soaking time necessary to obtain a substantial shift of T_m increased dramatically as the annealing temperature decreased. The giant shift of T_m determined by dielectric studies of ceramic samples was confirmed by X-ray diffraction and heat capacity studies of NLN-5 powder. In the as-sintered NLN-5 ceramics dielectric studies give $T_m \approx 360\ ^0C$. This value corroborate the literature data [1] and agrees well with anomalies in the temperature dependencies of the lattice parameters. In the annealed NLN-5 ceramics T_m increases up to $\approx 420\ ^0C$ while for the annealed NLN-5 powder, an orthorhombic phase is observed in the temperature range 20-390 °C; a pure cubic phase is seen above 460 °C while in the temperature range 400-450 °C orthorhombic and cubic phases coexist. According to both dielectric and X-ray diffraction data, heating of the samples up to 500 ^0C restores the initial value of phase transition temperature. The increased values of T_m remain stable at least for several months providing the annealed samples are stored at room temperature.

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The Application of Wang-Landau Algorithm for Simulation of Ferroelectrics

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The Ising model is widely used for simulation of phase transitions in ferroelectrics [1, 2]. But it is a satisfactory approach only if the ferroelectric has two possible directions of polarization (e.g. KDP). In the general case, the number of possible orientation states depends on the paraphase symmetry and can be more than two [3]. In the works [1, 2], the equilibrium properties are simulated for a predetermined crystal lattice. However, the lattice type and the crystallographic parameters could be changed under the influence of temperature, pressure and external electric fields. The equilibrium lattice type should be determined by a condition of free energy minimum. But the standard Metropolis algorithm does not allow calculating a partition function [4].

In this work, we apply the Wang-Landau algorithm [5] for simulation of phase transitions in ferroelectrics. The main advantage of this algorithm is that thermodynamic state functions (free energy, entropy etc.) can be calculated by means of one simulation in a wide range of temperatures. The Wang-Landau algorithm performs a random walk in the phase space to obtain the density of states. For models with two different types of interactions, the joint density of states should be obtained by two-dimensional random walk, but it requires huge computational time. The method for speed up the joint density of states calculations was developed in this work.

We use 6-state and 8-state Potts models with considering the competing influence of exchange and dipolar interactions. For these models, the values of free energy for different lattice types and crystallographic distances were calculated. The equilibrium lattice type is determined for different values of temperature. The phase diagram was built in dependence on the parameters of the competing interactions.

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Isosymmetrical Phase Transitions Between Deformationally Unstabl Sstates in Manganites

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Based on the phenomenological and statistical theories, the formation of phase states during rotational and Jahn-Teller phase transitions (PTs) in lanthanum manganites is investigated. Rotational orderings are characterized by two order parameters (OPs) - φ is transformed by the representation R_4^+, ψ - by M_3^+. Orbital ordering is characterized by OP χ, which transforms by M_2^+.

In manganites, the following sequence of high-temperature phases is observed: C → R → O → O ′, where C is the cubic phase, R is the rhombohedral phase with the symmetry group $R\bar{3}c$ ($\varphi\varphi\varphi$), O is the orthorhombic phase with the symmetry Pbnm ($\varphi\varphi\psi$), O′ is the rhombic phase, in which orbital ordering appears along with the rotational ordering. The phases O and O′ are isosymmetric. The orbital phase transition O → O′ is accompanied by a change in the main structural motive, as well as by significant ferroelastic deformations of the lattice. At the same time, in a number of compounds ($LaMnO_3$), the mentioned changes occur by a "jump", and in others ($PrMnO_3$, $NdMnO_3$) in a continuous manner.

The orbital phase transition is considered as a transition due to orientational ordering in three directions of tetragonally elongated octahedra due to the Jahn-Teller effect. It is shown that in such crystals condensation of OP ($00\chi_3$) will be accompanied by the appearance of a ferroelastic instability and by a "softening" of the modulus $(1/2)(c_{11} - c_{12})$. In this case, the PT will be of first order, accompanied by significant deformations. The interaction of rotational and orbital OPs is such that if there are two components of OP φ, the parameters ψ_3 and χ_3 interact bilinearly. Accordingly, the condensation of the critical parameter ψ_3 will lead to the appearance of the parameter χ_3. Thus, the condensate characterizing the O phase in the lanthanoid manganites will be $\varphi\varphi\psi_3\chi_3$.

The phase transition O → O ′, due to the proper orbital ordering, turns out to be a transition in an external field, which is determined by the product $\varphi\varphi\psi$. The condensate of OPs in the phase O′ is the same as in the phase O. Both phases have the same symmetry, i.e., are isosymmetric. In the phase O, the effect of the parameter χ_3 is insignificant, while in the phase O′ the main structural motif is formed by orbital ordering. The presence of an external field leads to the fact that under appropriate conditions, the phase transition from the phase O to the phase O′ becomes continuous.

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Determination of Temperature Dependence of Elastic Coefficients in Ferroelastics Under 4/m F 2/m Second-Order Phase Transition

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An analysis is made of the effect of the conservation of macrosymmetry in a polydomain crystal on the temperature dependence of the components of the elasticity tensor in crystals with a second-order phase transition 4 / m F 2 / m on the example of BiVO4. It is proved that the averaged elasticity tensor for two orientation states in the ferroelastic phase corresponds to the symmetry of the paraelastic phase. In order to preserve the macrosymmetry must occur redistribution of the values (an increase of one by decreasing the other) between the components of the elasticity tensor C_{11} and C_{22}, C_{13} and C_{23}, C_{16} and C_{26}, C_{44} and C_{55}, when the spontaneous deformation changes. The arithmetical mean of these components (Ciju) has a temperature dependence close to linear, with the exception of the region near the phase transition, which is well approximated by the logarithmic dependence (Fig.1.) The logarithmic dependence near Tc in the paraelectric phase was proposed by Levanyuk et al. [1].

Based on the obtained results of the study, we suggested the following types of temperature dependences of the components of the elastic tensor in the ferroelastic and paraelastic phases, which correspond well to the experimental data [2]:

$$C_{ij}^{m}(t) = k_1 + k_2 t + k_3 \ln(T_c - t)\,, \tag{1}$$

$$C_{ij}^{t}(t) = k_4 + k_5 t + k_6 \ln(t - T_c)\,. \tag{2}$$

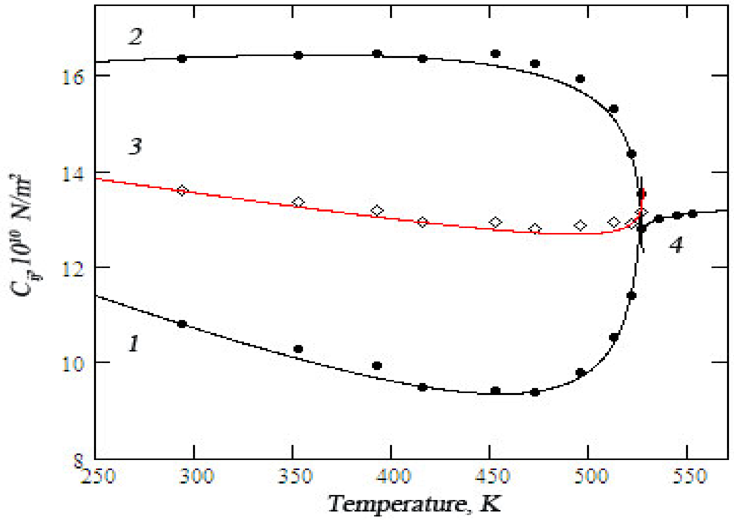

Fig.1. Temperature dependence of the elastic coefficients in BiVO$_4$ crystal; C_{11}^{m} (1), C_{22}^{m} (2), C_{11u} (3), C_{11}^{t} (4).

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Stochastic Model of Relaxors

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This report analyzes the role of stochastic effects in relaxors purposely to identify the main factors determining its anomalous properties. Random phase transition temperature distribution T_C^* on film thickness l, located in plane (x, y), due to fluctuation in the solid solution composition, has simulated by a differential equation for the order parameter η with a stochastic coefficient

$$\kappa \frac{d^2\eta(z)}{dz^2} + \left[\alpha + \xi(z)\right]\eta(z) = 0\,, \tag{1}$$

where κ is the correlation constant; $\alpha = \alpha_0\left(T_C - T\right)$ is the first coefficient of free energy expansion, proportional temperature T deviation from Curie temperature T_C of infinite homogeneous crystal; $\xi(z)$ is the random function, defining non-uniform film properties, chosen in the form [1]

$$\xi(z) = \xi_0\left(-1\right)^{n(z)},$$

where $n(z)$ is the integer random process with average $\bar{n}(z) = |z|/\left(2l_h\right)$, where l_h is the random function correlation radius. Equation (1) has solved together with non-random boundary conditions

$$\alpha_s\eta \mp \kappa \left.\frac{d\eta}{dz}\right|_{z=0,l} = 0\,, \tag{2}$$

where α_s is the parameter, describes the film interaction with medium. The stochastic boundary value problem (1), (2) has solved by the method, proposed in [2]. The mathematical expectation and dispersion of the phase transition temperature T_C^* to the relaxor state have determined as a random variables depending on a film parameters l, α_s and a random function parameters ξ_0, l_h.

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Phenomenological description of the sequence of phase transitions in intermetallic compounds

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The rare-earth intermetallic compounds RCo_2, (R = Gd, Tb, Nd, Ho, Er, Sm) crystallize into a cubic structure with the space symmetry group $Fd3m$. Most of these compounds have magnetic properties and experience a sequence of structural phase transitions (PT) from the cubic phase to the tetragonal and then to the orthorhombic one. The PT in the tetragonal phase is induced by an irreducible representation τ_5 of the G-point of the Brillouin zone with the space group $I4_1/amd$. The transition to the orthorhombic phase is induced by the same irreducible representation, which is two-dimensional, and the matrices of this representation form the symmetry group of the order parameter (OP) $L=C_{3v}$. Low-temperature PT in intermetallic compounds occurs with the appearance of spontaneous magnetization, and is induced by a three-dimensional irreducible representation τ_9 of the G-point of the Brillouin zone. This means that the thermodynamic potential describing structural and magnetic PT's should be a function of two interacting two-dimensional OP's with $L = C_{3v}$, describing structural PT and three-dimensional with $L = T_d$, responsible for the PT in a magnetically ordered state, that is, L- group should be $L = T_d \oplus C_{3v}$ and the composite OP is five-component. In [1] it was shown, that the low-temperature orthorhombic phase in RCo_2 compounds has the space symmetry group $Imma$ and the PT's sequence $Fd3m \rightarrow I4_1/amd \rightarrow Imma$. A structural phase transition from a cubic to a tetragonal phase occurs according to a two-dimensional OP, and only one component is different from zero in the tetragonal phase. The magnetic phase transition also occurs with the appearance of a single component OP. Using the method of effective potential, one can consider a model with two one-component OP's, while retaining all the characteristic features of the behavior of intermetallic compounds. Formally, one can assume that the parameter η is fully symmetric with the group $L= C_1$, and the symmetry of the magnetic order parameter is determined by the group $L= C_s$.

The phenomenological model with the group $L=C_1 \oplus C_s$, constructed by methods of the theory of catastrophes [2], has the form

$$\Phi = a_1\eta^2 + b_1\eta^3 + c_1M^2 + c_2M^4 + d_1\eta M^2 + d_2\eta^2 M^2 + a_2\eta^4 - aMH .$$

Model describes three phases that are different in symmetry: 1. $\eta = 0$, $M = 0$ — a high-symmetry phase; 2. $\eta \neq 0$, $M = 0$ — elastic phase; 3. $\eta \neq 0$, $M \neq 0$ — elastic and magnetic phase. The theoretical temperature dependences of the anomalous part of the heat capacity, as well as the magnetization of the external magnetic field, showed a qualitative agreement with experiment. Low-temperature PT in intermetallic compounds may be due to the interaction of the structural and magnetic sublattices of the crystal. The hysteresis observed on the field dependences of the magnetization in $ErCo_2$ [3] in the framework of the model can be interpreted as an isostructural PT.

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Phase Transitions in $(NH_4)_2KZrF_7$

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A structural complex in the form of a pentagonal bipyramid is realized in the isostructural fluorine compounds $(NH_4)_3HfF_7$ and $(NH_4)_3ZrF_7$. The crystals have the structure of an ordered perovskite (elpasolite) at ambient conditions with a cubic face-centred lattice (sp. gr. $Fm3m$) in which the F ions form a pentagonal bipyramid around Zr(Hf), having 24 equivalent orientations. [1, 2].

Recently, we have studied heat capacity, crystal optical properties and susceptibility to hydrostatic pressure of $(NH_4)_3HfF_7$ and revealed that crystal undergoes the succession of six structural phase transitions of nonferroelectric nature [2]. At ambient and high pressure, thermal properties of $(NH_4)_3HfF_7$ investigated using DSC and DTA under pressure revealed seven anomalies associated with the successive phase transitions similar to those that we found recently in $(NH_4)_3ZrF_7$. Birefringence and optical twinning studies were able to detect only four phase transitions with the following change of the point groups: $Fm3m \leftarrow T_0 \rightarrow$ cub. $\leftarrow T_1 \rightarrow$ mmm (1) $\leftarrow T_2 \rightarrow$ mmm (2) $\leftarrow T_3 \rightarrow$ mmm (3) $\leftarrow T_5 \rightarrow$ 2/c in $(NH_4)_3HfF_7$. Similar differences between the thermal and optical data were also observed for $(NH_4)_3ZrF_7$. A change in the chemical pressure associated with the Hf → Zr substitution was accompanied by the following:

1) an insignificant change in the phase transitions temperatures
2) different symmetry succession of the distorted phases observed in optic studies;
3) a decrease in the total entropy change;
4) a lower resistance of distorted phases to external pressure.

The substitution of ammonium with potassium could lead to unusual results such as the appearance of new phases, the wedging out of old ones and even the appearance of polar phases. Thus, it was easy for us to set a problem with cation substitution in heptafluorozirconate.

First of all, we obtained and studied the crystal $(NH_4)_2KZrF_7$. Two heat capacity anomalies near 320K in heating and one in cooling were detected by the DSC method. The existence of these two heat capacity anomalies was confirmed by adiabatic calorimetry and dilatometry, where measurements were performed in a heating mode only. Optical and X-ray studies also have shown the presence of distortion of the structure near 320 K, it is shown that the structure changes from cubic ($Fm3m$) to tetragonal ($P4_2/nmc$) and remains down to 100K.

Thus, it was found that partial substitution of ammonium with potassium lead to a significant reduction in a number of phase transitions. At the moment, studies are ongoing.

Acknowledgment. This work was supported by Russian Foundation for Basic Research (Grant N 18-02-00269)

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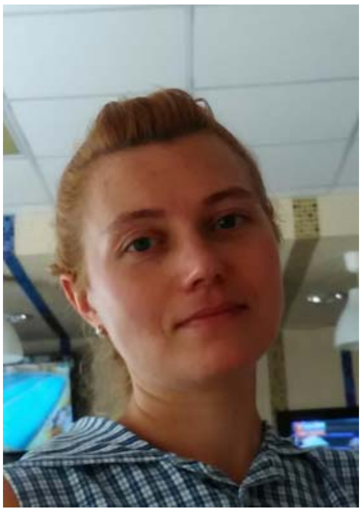
III. Structure and Physical Properties



Temperature-Induced Changes in the Structure of $PbYb_{1/2}Nb_{1/2}O_3$ Ceramics with Differing Ordering Degree of Yb and Nb Cations

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Compounds crystallizing in the perovskite structure are among the most intensely studied materials in solid state chemistry and physics [1-3]. The physical characteristics of binary perovskites $Pb(B1_xB2_{1-x})0_3$ (B1 = Sc^{3+}, In^{3+}, Yb^{3+}, B2= Nb^{5+}) with x=1/2 are strongly dependent on the chemical ordering i.e. the character of of the B-site cations distribution at the equivalent sites of the perovskite lattice.

$PbYb_{1/2}Nb_{1/2}O_3$ (PYN) tends to crystallize in an ordered state [4]. The degree of ordering is usually estimated by a long-range ordering degree parameter s according to the data of X-ray powder diffraction. Recently it was found out that it is possible to use high-energy mechanoactivation for changing the degree of ordering, and, accordingly, the electrophysical characteristics of PYN [5,6].

We carried out X-ray powder diffraction and dielectric permittivity ε studies in the temperature range 20-350 ^{O}C of three polycrystalline PYN samples, denoted hearafter as S1, S2 and S3, which were obtained by mechanochemical synthesis at different conditions. X-ray studies confirmed the formation of perovskite structure for all the three samples. Lattice constants and long-range ordering degree s were determined by the Rietveld method.

X-ray diffraction data for the sample S1 have shown the formation of PYN with totally disordered Yb^{3+} and Nb^{5+} cations (s=0). According to the measured ε(T) curves, this sample exhibited a relaxor-like dielectric behavior. Temperature dependence of lattice parameters also showed the presence of a diffuse phase transition and correlated perfectly with dielectric data. Samples S2 and S3 were characterized by the long -range ordering degree values s= 0.48 and 0.62. They exhibited non-diffused and frequency-independent ε(T) maxima at temperatures $T_m \approx 170$ and 250 ^{0}C respectively. The T_m values of all the three samples studied are in good correlation with the T_m-s^2 phase diagram plotted for PYN ceramics in which disordering was achieved by Li-doping [2].

Acknowledgment.This work was supported in part by RFBR (project 17-03-01293_a) and by the Ministry of Education and Science of the Russian Federation (research projects. 3.1649.2017/4.6 and 17-02-00616\18).

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Transition of Weak Signals via Ferroelectric Capacitor with Negative Capacitance

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In the report presented we discuss behaviour of ferroelectric capacitor with negative capacitance connected in series with resistance under the action of external voltage.

A proof-of-concept demonstrations of negative capacitance effect in a nanoscale ferroelectric-dielectric heterostructures were described in articles [1] and [2]. Such heterostructures possess by the following dependence of voltage on it from its charge q [1, 2]:

$$U(q) = -\alpha \cdot q + \beta \cdot q^3 , \ \alpha > 0 , \ \beta > 0 . \qquad (1)$$

Due to formula (1) evolution of the system under investigation in dimensionless time τ obeys to the next ordinary differential equation for dimensionless charge x(τ):

$$\frac{dx}{d\tau} - x + x^3 = u(\tau) , \quad x(0) = x_0 . \qquad (2)$$

We suppose that dimensionless external voltage u(τ) is quite small therefore we shall find solution of equation (2) in the framework of theory of perturbations namely $x(\tau) = x^{(0)}(\tau) + x^{(1)}(\tau) + \ldots$ where

$$\frac{dx^{(0)}}{d\tau} - x^{(0)} + x^{(0)3} = 0 , \quad x^{(0)}(0) = x_0 . \qquad (3)$$

and

$$\frac{dx^{(1)}}{d\tau} + (-1 + 3 \cdot x^{(0)2}) \cdot x^{(1)} = u(\tau) , \qquad x^{(1)}(0) = 0 . \qquad (4)$$

Using equations (3) and (4) we consider response of the system on both determinate and stochastic input voltage u(τ).

Acknowledgment. This work was supported by Russian Foundation for Basic Research (Grant N 18-08-01356-a)

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Dielectric hysteresis in 2-Methylbenzimidazole Single Crystals and Textured Spherulite Films

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2-methylbenzimidazole (MBI) exhibits ferroelectricity at room temperature [1]. Coercive field and spontaneous polarization are $E_c \sim 3$ V/μ and $P_s = 5$ μC/cm^2 respectively. MBI structure belongs to pseudo-tetragonal symmetry $P4_2/n$ (Pn). Spontaneous polarization caused by the ordering of protons in hydrogen bonds chains N – H ••• N, lies in a plane perpendicular to the pseudo-tetragonal axis.

The work is devoted to the study and comparison of dielectric hysteresis loops in MBI single crystals and MBI spherulite films. The loops were measured in the Sawyer-Tower circuit in fields up to 17 V/μ (for films) in the frequency range 25-3000 Hz at temperatures of 290-380 K. Loops were simulated in Janta model [2]. It is shown that heating leads to a decrease in the activation field of the domain wall motion.

Polarization microscopy, XRD analysis and AFM showed that MBI films consist of spherulite blocks (Fig. 1a). Each block is a split crystal and consists of needle-shaped crystallites elongated along the pseudo-tetragonal axis, growing radially from the center of the block. The films were grown on substrates with preliminary deposited interdigital systems (IDS) of electrodes. Films could be covered by the top electrode, so polarization switching was observed both for out-of-plane and in-plane electric field orientation. In the second case, the loop (Fig. 1b) is quite similar to that observed in a single crystal, but due to the difference in crystallite orientations, the remnant polarization is less than 5 μC/cm^2, and the P_r (E_{max}) dependencies are shifted towards stronger fields.

a) b)

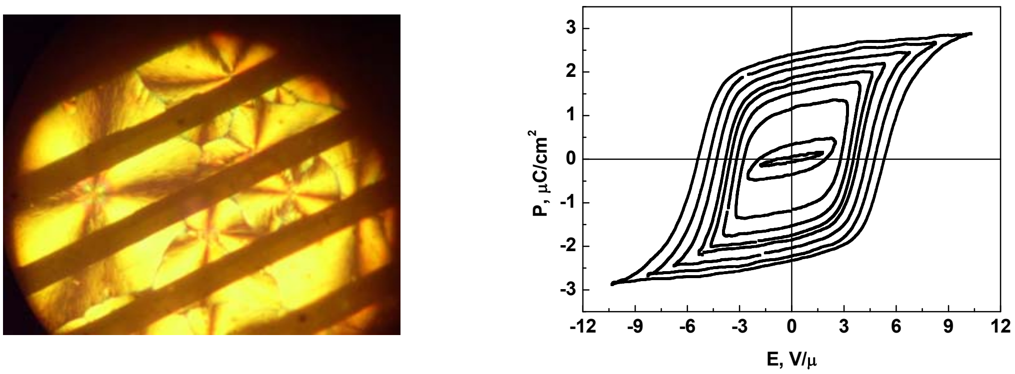

Fig. 1. a) Image of spherulite MBI film observed in the polarization microscope with crossed polarizers. The dark bands correspond to the gap between the electrodes of a width of 20 μ. b) Dielectric hysteresis loops in MBI film, measured for in-plane electric field orientation. $T = 291$ K, $f = 25$ Hz.

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Dielectric and Switching Properties of Barium Titanate Type Layered Structures in Weak and Strong Electric Fields

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Barium titanate $BaTiO_3$ is one of the widely popular ferroelectric materials. To improve quality the ferroelectric properties of barium titanate and their range it is possible to create multilayer thin-film structures using other perovskite-like materials. The mechanical stress occurring at the interface of the adjacent layers leads to a significant change in all dielectric properties of the obtained multilayer structures. In this paper, layered structures with alternating layers of barium titanate and other non-ferroelectric material, which also had a crystal lattice with a perovskite structure, were investigated. Two types of samples were studied: with alternating layers of barium titanate/barium zirconate and barium titanate between two layers of strontium titanate. In both cases, the mechanical stresses in the contact plane of the layers due to the difference in the crystal lattice parameter of the components led to a significant increase of the phase transition temperature compared to the single-component barium titanate.

The studies of the electro-physical properties of these structures in external electric fields with sinusoidal and rectangular waveforms have shown the presence of a sufficiently large value of spontaneous polarization, coercive and internal bias fields. Analysis of switching currents for the weak and strong fields showed that there are two regimes of switching - activation ("creep motion") and non-activation ("slip region"). The value of the threshold field separating these areas corresponds to the coercive field and also decreases when approaching the Curie point.

In the study of switching currents in weak fields, it was found that the integral characteristics of switching, and hence the speed of the domain boundaries do not correspond strictly exponential dependence on the field strength. Consequently, the dependence of the switching current (and the velocity of the domain boundaries) on the electric field strength has a dynamic coefficient μ, the value of which is less than one and almost does not change when approaching the phase transition point.

For the region of strong fields, the mobility of the domain walls at various temperatures is calculated on the basis of the switching time. As the temperature increases, the switching time increases, which means a decrease in the mobility of the domain walls associated in our opinion with a critical deceleration of the polarization relaxation near the Curie point.

Acknowledgment. This work was supported by Russian Science Foundation (project No. № 17-72-20105).

Electric Properties of Magneto Resistive Composites Based on $La_{0.7}Sr_{0.3}MnO_3$

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Magneto-resistive heterogeneous materials, synthesized near a percolation threshold on the based on perovskite - strontium lanthanum manganite $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and the second phase (I), have interesting physical properties also have the practical prospects of application, for example, as sensitive sensors of constant magnetic fields. The cause of extrinsic magnetoresistance (MR) and magnetodielectric properties (MD) in such composite materials is spin-dependent inter-granular tunneling [1, 2]. It should be noted that spin-dependent tunnel effects in such composites occur with a wide temperature range 0-360 K, unlike its intrinsic magneto-resistive effect of manganites, which is observed near temperature of ferromagnetic-paramagnetic phase transition.

Composite structures with connectivity 3-0 near percolation threshold, based on LSMO and dielectric phase, have been synthesized in our work in which such compounds as SiO_2, GeO_2, Al_2O_3, BaO, WO_3, $Li_4P_2O_7$, NiO, CuO, ZnO, Sb_2O_3, $SrTiO_3$, $SrFe_{12}O_{19}$ and other oxides have been studied. The X-ray diffraction showed the existence of two main phases – manganite, and dielectric phase as the second one. Ceramic composites such as LSMO/Me have also been made as a result of self-propagation high-temperature synthesis with the use of silver nitrate, where Me is metal phase - Ag with various ratio of components. The study of volt-ampere characteristics (VAC) of the synthesized composite materials of a series of LSMO/GeO_2 in magnetic fields strength up to 15 kOe has shown nonlinear characteristics of structures near percolation threshold that is 85%LSMO/15%GeO_2. This fact corresponds to the findings [4], where VAC parabolic dependence is noticed in case of plenty of tunnel transitions. Values of electric current, caused by spin-dependent tunneling of charge carriers, have the linear nature of dependence on strength of external magnetic field. Long- term tests of magneto-resistive properties in aggressive environment (with water salinity of 35 ppm) of glass composites with GeO which electrical resistance is 3-5 Ω have shown high stability of magneto-resistive properties, with insignificant shunting because of sea water conductivity.

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Investigation of the Influence of Volume on the Surface of Ferroelectric Systems

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The electrophysical properties of ferroelectric films mainly depend on the morphology of the surface, its crystallinity, density, crystallographic orientation, and other structural properties, which, in turn, depend on the technological parameters of film formation. Structural studies of samples of ferroelectric films make it possible to select the optimal modes of their formation [1-2]. Thus, the study of the surface of ferroelectric systems is an urgent task.

In this work, to describe the surface of ferroelectric polymer films, we used a two-dimensional model, which is a system of freely-articulated chains, each of which is a sequence of hinged-connected rigid segments arranged parallel to the surface [3]. The order parameter was determined as the average cosine of the angle between the directions of the director and the instantaneous direction of the axis of the segment, taking into account the interaction of the selected surface chain with the rest of the chains in the volume.

Since this influence is different, the mean field theory was used. The aim of the work was to determine the order parameter depending on temperature, mean field strength, persistent length, and interchain interaction constants. This problem was solved analytically in normal coordinates. Formulas for calculating the free energy for a two-dimensional polymer film on the surface are obtained. The equilibrium value of the order parameter was determined from the condition of minimum free energy.

The dependences of the order parameter for an infinitely extended system on the interchain interaction constants, on the values of the persistent length and on the parameters of the mean field are given. The values of parameters of interchain interactions at the phase transition point are also calculated. The magnitude of the interaction is determined by the distance between the layers of the polymer system. It is shown that with a decrease in the distance between the layers, the average field value decreases, which leads to a decrease in the phase transition temperature.

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Dielectric properties of ferroelectric ceramics with the structure of Aurivillius phases

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Great interest in layered perovskites with the structure of the phases of Aurivillius (FA) is due to the prospect of their practical use as elements of nonvolatile ferroelectric memory (FeRAM) devices, ionic conductors, catalytic compounds, electroluminescent thin films, and multiferroics. Such a wide area of potential application of FA is associated with a unique set of physical characteristics of these compounds.

The purpose of the work was to study the effect of different concentrations of nickel in layered perovskite $Bi_6Ti_3Fe_{2-x}Ni_xO_{18}$, (x=0; 0,1; 0,2; 0,3; 0,4) with the number of perovskite-like layers equal to 5, the dielectric properties in the temperature range from 25 °C to 600 °C.

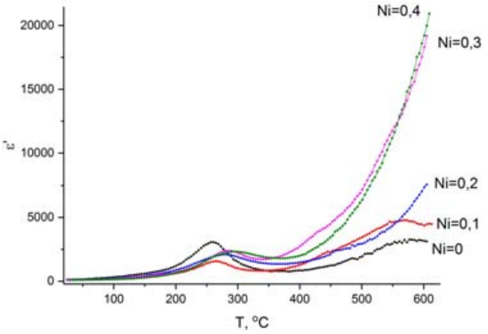

Fig. 1 Dependences of ε′(T) for $Bi_6Ti_3Fe_{2-x}Ni_xO_{18}$, with different contents of x (Ni) at 1 kHz

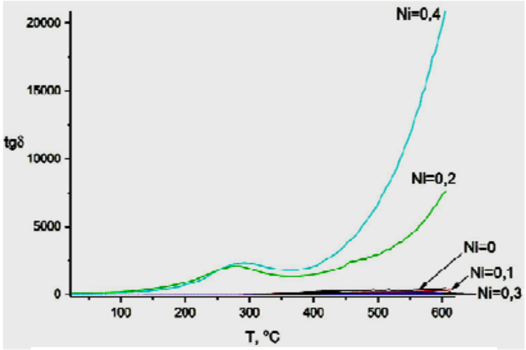

Fig. 2 Dependences of tgδ(T) for $Bi_6Ti_3Fe_{2-x}Ni_xO_{18}$with different contents of x (Ni) at a frequency of 1 kHz

The analysis of the obtained dependences of the dielectric constant showed a shift of the maximum to the region of high temperatures with increasing nickel concentration in the composition. The data obtained correlate well with the results of studies of the dielectric loss tangent tgδ.

Testing the feasibility of the Curie-Weiss law showed that in a wide temperature range in the vicinity of the maximum dielectric constant this law is not fulfilled. This fact indicates that the phase transition is blurred. To describe it, a model of fluctuations in the composition of Smolensky-Isupov was chosen. Within the framework of the model, an estimate was made of the degree of blurring of the phase transition depending on the nickel concentration in the composition, with the growth of which the blurring becomes larger. The volume of the critical nucleus of the polar region is determined to be 10^{-22} cm^3, which is close in order of magnitude to the value of the Känzig volume.

This work was supported by the Russian Foundation for Basic Research, grant No. 18-52-00039.

Dielectric properties of $Sr_{2+x}Bi_{4-x}Ti_{5-x}Ta_xO_{18}$ ferroelectric ceramics

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The aim of this work was to study the dielectric properties of $Sr_{2+x}Bi_{4-x}Ti_{5-x}Ta_xO_{18}$ layered perovskite (x = 0, 0.2, 0.4) at various frequencies in a wide temperature range.

The investigated samples with the general formula $Sr_{2+x}Bi_{4-x}Ti_{5-x}Ta_xO_{18}$ were obtained by standard two-stage ceramic technology. For the synthesis, $SrCO_3$; Bi_2O_3; TiO_2; Ta_2O_5. Analysis of the samples by X-ray diffraction showed that all samples are single-phase and belong to the orthorhombic symmetry group. The number of perovskite-like layers is m = 5. The temperature dependences of the real ε ', imaginary ε' 'part of the dielectric constant and the tangent of the dielectric loss angle tgδ were obtained by the method of dielectric spectroscopy. Temperature dependencies of ε 'and ε' 'at various frequencies for the composition with x=0.2 are presented in Figures 1 and 2, respectively.

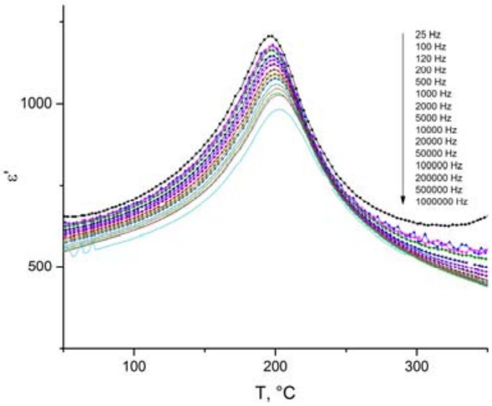

Fig. 1 Dependences of ε´(T) for $Bi_6Ti_3Fe_{2-x}Ni_xO_{18}$, with x=0.2 at various frequencies

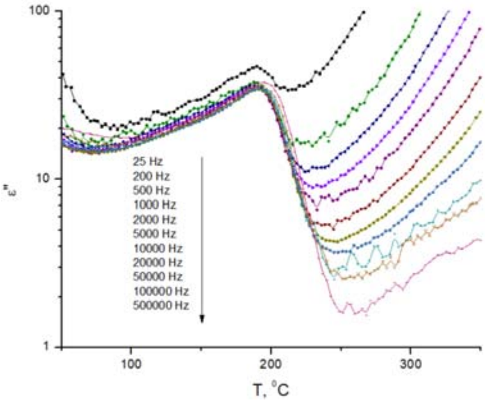

Fig. 2 Temperature dependences ε" for $Bi_6Ti_3Fe_{2-x}Ni_xO_{18}$ with x=0.2 at various frequencies

It was found that, with an increase in the concentration of Ta ions, there is a blurring of the phase transition and a shift of the transition to the region of low temperatures. The parameters of the Curie-Weiss law and the effect on them of changes in the concentration of Ta ions are determined. Found that below the temperature of the Burns clearly manifested low-frequency $1/f^{\alpha}$ - noise. The dependence α(T) is determined in the temperature range of the ferroelectric and paraelectric phases, which indicates that the system becomes less dynamically heterogeneous in the paraelectric phase.

This work was supported by the Russian Foundation for Basic Research, grant No. 18-52-00039.

Peculiarities of Polarization Behavior in Ferro electric Solid Solution $0.75PbTiO_3$ - $0.25PbCd_{1/3}Nb_{2/3}O_3$

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Ferroelectrics with a diffuse phase transition are of particular interest to science and technology. Blurring, as a rule, occurs in ferroelectrics with a complex perovskite lattice, as well as in solid solutions of ferroelectrics. One of the manifestations of blurring is the "broadening" of the peak of the dielectric constant at the phase transition, which can reach hundreds of degrees. The blurring of a phase transition in a certain way can affect other physical properties of a substance, for example, polarization.

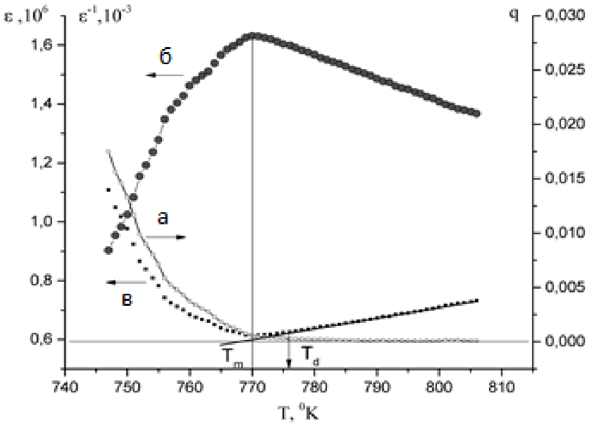

Fig. 1 Temperature dependence of local order parameter q on (a) in comparison with temperature dependences of ε (b) and ε^{-1} (c).

Therefore, the establishment of features of polarization in such substances is an urgent task. The purpose of this work was to determine the temperature dependence of the local order parameter in the $0.75PbTiO_3$ - $0.25PbCd_{1/3}Nb_{2/3}O3$ solid solution obtained by the ceramic technology. On the temperature dependence of the dielectric constant in the transition region, a peak broadening is observed (Fig. 1, b). The blurring of the phase transition was interpreted in terms of the composition fluctuation model. According to this model, in the solid solution there are local polar regions, whose T_C temperatures are statistically distributed over the sample volume. In this connection, there is a "blurring" of the phase transition. The blur parameter, estimated for our composition, has the value $\sigma = 25$ K. The dependence $\varepsilon^{-1}(T)$ shows the region where the linear Curie-Weiss law does not hold. The Burns temperature Td = 776 K, at which the deviation from the linear law begins, is the temperature at which the polar regions begin to form. The root-mean-square polarization in the blur region is characterized by a local order parameter q. To analyze the dependence of q(T), an approach was used that allows one to determine the dependence of polarization on temperature, using data obtained during measurements of the dielectric constant, i.e. $\varepsilon^{-1}(T) = (T-T_0)/C_{CW} + f(T)$, where $f(T) = \varepsilon_0 \gamma q(T)$, γ is the thermodynamic coefficient. Since the γ coefficient cannot be determined from measurements of the dielectric constant, the function f (T) was extrapolated to absolute zero temperatures, and the ratio of f (T) at some temperature to the value at absolute zero was considered as a measure of the local order parameter. The dependence q (T) is shown in Figure 1, a. It can be seen that the rms polarization is different from zero not at the temperature of the maximum dielectric constant, but at the Burns temperature of ~ 776 K, then it slowly increases with decreasing temperature.

This work was supported by the Russian Foundation for Basic Research, grant No. 16-02-00072.

IV. Heterogeneous, Glassy and Incommensurate systems

Distribution of Polarization in Thin Films with Incommensurate Ferroelectric Phase

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Currently, the great progress has been achieved in the field of processing single-crystal thin-film structures. In this regard, the task of developing and manufacturing new equipment and technical devices for various purposes based on these structures becomes realistically achievable. In this context, the expediency of developing theoretical studies on low-dimensional physical phenomena in these objects greatly increases. Among the mentioned materials, ferroelectric thin films play a significant role. Their properties including the occurrence of phase transitions significantly change when the thickness of these materials approaches nanoscale level. The latter concerns not only the ordinary phase transformations, but also the transitions to the so-called incommensurate phase in samples with nanoscale thickness, wherein the modulation period of the order parameter, obviously, should be sensitive to the size effects.

In the present work, the influence of size effects on phase transitions to an ncommensurate phase with periodically changing the spontaneous polarization vector in single-crystal ferroelectric thin films has been investigated. It was shown that fixing of spontaneous polarization vector on the surface of a ferroelectric layer leads to limiting the number of acceptable equilibrium states in the polarization distribution in the sample with finite sizes and to the emergence of the transitions between the states. Temperature-dependent film thickness intervals with even or odd distribution of spontaneous polarization vector were determined. It was demonstrated that the variation of ferroelectric film thickness and temperature provides practically important conditions for stabilizing symmetric or antisymmetric states with respect to polarization distribution in thin ferroelectric films with incommensurate phase. Possible applications of the considered effects were analyzed.

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Phase Transitions in Confined KDP, ADP and CDP

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Intensive development of nanotechnologies is a significant stimulus to clarify patterns of the size effect in systems with ultradisperse particles of different topology and dimension in recent years. As an example of such systems, consider composite materials that are polar dielectrics embedded in porous structures having a branched network of through pores.

Interaction of embedded material and matrix leads to the shift of phase transition temperature T_C. However the data concerning displacement of T_C, obtained by different authors for the same embedded materials, are quite different [1-3].

The present work is devoted to comparative study of restricted geometry impact on transition temperature in the embedded particles of potassium dihydrogen phosphate (KH_2PO_4 - (KDP), cesium dihydrophosphate (CsH_2PO_4 - CDP) and ammonium dihydrogen phosphate ($NH_4H_2PO_4$ - ADP) into porous matrix with different average pore diameters. The KDP, CDP and ADP crystals have a similar chemical composition, but differ in the magnitude of pressure coefficient ($\gamma = dT_C/dP$), values of piezoelectric modulus and in the temperature coefficient of linear expansion.

The composite materials under study were synthesized by embedding of ferroelectrics KDP and CDP and antiferroelectric ADP in porous glass matrixes with an average size of through pores of 7, 46 and 320 nm from corresponding aqua solutions. An increase of T_C was observed for embedded particles in comparison with appropriate bulk materials. Some possible mechanisms of the influence of “restricted geometry” on the Curie temperature are discussed. Estimates of T_C shifting (ΔT_C) as a result of the "negative pressure effect" caused by elastic stresses in implanted particles are presented together with estimates of ΔT_C caused by the electric field owing to the piezoelectric effect in the KDP and ADP particles in the paraelectric phase.

The possibility of using the Ising tunnel model [4] to explain the experimental results is also discussed.

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Properties of $BaTiO_3/KNbO_3$, $SrTiO_3/KNbO_3$, and $PbTiO_3/KNbO_3$ Ferroelectric Superlattices

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Low-dimensional structures in which new physical phenomena with no analogues in the 3D world have been discovered and which are promising for practical applications attract a great attention. In this respect, the study of periodic quasi-two-dimensional systems – ferroelectric superlattices (SL) – is of considerable interest, too.

So far, the most thoroughly studied ferroelectric superlattices were superlattices which had no double layers at the interface of contacting materials and which were macroscopically electrically neutral. Investigations of $SrTiO_3/LaAlO_3$ heterostructures have revealed interesting phenomena that arise in structures with electrical double layers as a result of a variation in the electrostatic potential near the interface. These effects include the appearance of electrically conductive layers, their magnetism and even superconductivity [1].

In this work, the physical properties of [001]-oriented short-period $(BaTiO_3)_1(KNbO_3)_1$, $(SrTiO_3)_1(KNbO_3)_1$, and $(PbTiO_3)_1(KNbO_3)_1$ superlattices, in which the presence of charged layers of KO^- and NbO_2^+ induces the perturbation of electrostatic potential, were studied using the first-principles calculations. The calculations were performed within the density-functional theory using the ABINIT software package.

First, the calculations have proven that no metallization of the contacting layers in the superlattices occur: the conduction band is separated from the valence band by an energy gap of several eV. Since the sequence of layers has no mirror symmetry, the superlattices are always polar. The search for the ground state of their structure was carried out in the traditional way [2,3]. It turned out that in all SLs, the high-symmetry *P*4*mm* phase exhibits the ferroelectric instability with respect to the in-plane polar distortions, and moreover there is additional antiferrodistortive instability in the $SrTiO_3/KNbO_3$ SL. The ground states of *Cm*, *Pc*, and *Cm* symmetry were obtained for the $BaTiO_3/KNbO_3$, $SrTiO_3/KNbO_3$, and $PbTiO_3/KNbO_3$ SLs, respectively. For these structures, the polarization and piezoelectric tensor components were calculated. In $BaTiO_3/KNbO_3$ and $SrTiO_3/KNbO_3$ SLs, the polarization vectors are strongly inclined to the plane of superlattice and their magnitudes are 0.339 and 0.289 C/m^2, respectively. In the $PbTiO_3/KNbO_3$ SL, the polarization is slightly deviated from the normal direction and its magnitude is 0.581 C/m^2. The most interesting result is that the highest piezoelectric coefficients in all three SLs are related to the in-plane strain. The values of e_{11} and e_{22} coefficients for $BaTiO_3/KNbO_3$, $SrTiO_3/KNbO_3$, and $PbTiO_3/KNbO_3$ SLs are 7.8, 10.1, and 11.5 C/m^2, respectively. Thus, a decrease in the symmetry of the superlattice resulting from the in-plane ferroelectric instability in SLs leads to interesting piezoelectric properties of these SLs.

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Phase Transitions in Rb_2ZnCl_4 Particles under Restricted Geometry Conditions

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The physical effects in nanosized ferroelectrics have been studied to some extent at present. At the same time, the problems associated with the appearance of an incommensurate phase, its temperature evolution, and the transition to a commensurate polar phase under so called restricted geometry conditions have not been practically investigated.

Therefore the purpose of present work is study of structure, calorimetric and dielectric properties of Rb_2ZnCl_4-SiO_2 nanocomposites.

The matrix nanocomposites of Rb_2ZnCl_4 - SiO_2 system were prepared by embedding of Rb_2ZnCl_4 salt into porous glasses with average diameter of through pores near 320, 160, 46 and 23 nm from saturated aqueous solution (Abbreviations of the samples are RS-23, RS-46, RS-160 and RS-320). X-ray analysis (Cu-Kα radiation) showed that the crystallized in porous material and bulk Rb_2ZnCl_4 possess identical crystalline structure. Results of dielectric and calorimetric measurements are presented in Fig. 1 and Fig. 2.

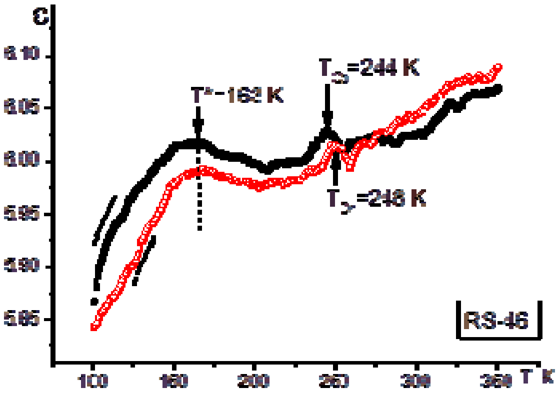

Fig. 1. The temperature dependence of the dielectric permittivity for RS-46 sample

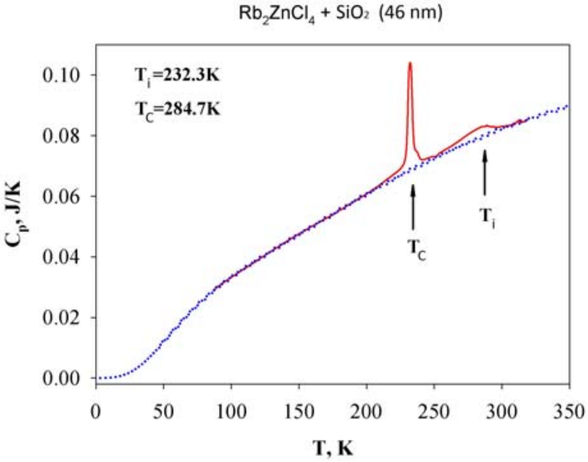

Fig. 2. The temperature dependence of the heat capacity for RS-46 sample

Two anomalies of dielectric permittivity (ε) at temperatures of about 160 and 250 K for RS-23, RS-160 and RS-320 samples were found (Fig. 1). The maximum of ε corresponding transition to incommensurate phase at $T_i \approx 300$ K is not seen in Fig. 1. However the diffused maximum of heat capacity C_p near T_i is observed (Fig. 2). The distinct peak of C_p near 232 K is accompanied by the step-like anomaly of ε (≈ 244 K). These anomalies are associated with the ferroelectric phase transition that in the single crystal of Rb_2ZnCl_4 is realized at $T_C \approx 192$ K. A significant increase in the temperature of the ferroelectric phase transition in under restricted geometry conditions probably is due to mechanical stresses in Rb_2ZnCl_4 particles caused by the difference in the temperature coefficients of the linear expansion of the matrix and the embedded material.

The diffused maximum of ε near T* = 160 K is not accompanied by any peculiarities in the $C_p(T)$ dependence. The origination of this maximum of ε is discussed.

Electromechanical and Dielectric Anomalies on the Electric Field Dependences of the Relaxor Ferroelectrics

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Solid solutions of the relaxor ferroelectrics $PbMg_{1/3}Nb_{2/3}O_3$ (PMN), $PbZn_{1/3}Nb_{2/3}O_3$ (PZN), $PbNi_{1/3}Nb_{2/3}O_3$ (PNN) and classical ferroelectric $PbTiO_3$ (PT) are of a great interest due to the high values of piezoelectric and dielectric parameters [1-3]. Electric field dependences of the longitudinal strain and dielectric constant are the main functional characteristics for applications of materials in actuators and tunable devices. One feature of the dielectric constant dependence on electric field of ferroelectric materials is the presence of minima which appear with increasing of electric field value (in bipolar regime). These anomalies were observed on the dependences of different ferroelectric systems [4,5]. The aim of this work was a detailed study of the anomalies of electromechanical and dielectric responses of relaxor-based ceramics in electric fields.

Object of the study were the ceramics of system mPMN - nPNN - yPZN - xPT (m = 0.1298-0.4844, n = 0.1266-0.4326, y = 0.0842-0.130, x = 0.25-0.40), modified by 5 mol. % of barium which were prepared by solid state synthesis and were sintered by conventional ceramics technology. Dependences of the dielectric permittivity and the longitudinal strain on electric field were measured with a help of the testing bench which includes LCR-meter Agilent 4263B and a galvanomagnetic dilatometer with a digital indication of readings. Measurements were made in quasi-static mode range of -15 – +15 kV/cm in bipolar mode and 0 – +15 kV/cm in unipolar one.

The evolution of electric field dependences of the dielectric permittivity and the longitudinal strain with increasing of PT content from relaxor-like to typical for classical ferroelectrics was shown. The existence of plateau-like anomalies on the dependences of heterophase ceramics ($x \approx 0.30 - 0.35$) at E ~ 5 kVcm has been established. The origin of these anomalies is a termination of non 180°- domain switching due to high mechanical strains caused by electric field induced phase transition from the heterophase ($Psc + T$) to single-phase (T) state [6]. It was shown that electric field in unipolar regime does not lead to the formation of anomalies of dielectric and electromechanical properties. The latter feature should be taken into account when using materials based on relaxor ferroelectrics in actuator technique.

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Harmonic Analysis of the Repolarization Current in the Solid Solutions $(Rb_{1-X}K_X)_2ZnCl_4$

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In the physics of ferroelectric phenomena, both from the standpoint of fundamental science and from an applied point of view, the study of the laws of switching the domain structure under the influence of various external influences plays an important role. There are many approaches to the description of the nonlinear dependence of polarization on the voltage value and to the construction of the model of repolarization of ferroelectric materials [1, 2], but none of them is based on the use of Fourier series. Although, as is known [3], it is a harmonic analysis of the process of repolarization of ferroelectric materials is the most informative and complete for the study of nonlinear properties of ferroelectric materials. In [4], the possibilities of this method were significantly expanded by separation of the contributions to the harmonic components amplitudes of the Sawyer-tower scheme output signal from the processes of repolarization of the studied samples and processes associated with dielectric losses that arise when domain boundaries are switching.

This allowed to trace a number of patterns of domain dynamics in the studied samples, which are not registered by other methods. According to this method the current of complex periodic shape occurs in the studied samples, which density $J_x(t)$ is described by a Fourier series, due to the application of an alternating electric field to samples with the amplitude sufficient for the complete monodomenization of the sample.

The dependence $J_x(t)$ includes two components $J_c(t)$ and $J_g(t)$. The first component is due to the capacitive current density, and the second component is due to the conductivity current density. For all measured samples, the contributions of the harmonic components of the Sawyer-tower scheme output signal $J_{cc}(t)$ and $J_{gg}(t)$, respectively, in $J_c(t)$ from the processes of repolarization of the studied samples and in $J_g(t)$ from the processes associated with dielectric losses arising when switching domain boundaries are experimentally separated. For all studied samples dependences $J_{cc}(t)$ and $J_{gg}(t)$ coincide in the range of normalized time $щ_0t$ from pn to p/2+pn, where n=0,1,2,..., at other times $J_{cc}(t)=-J_{gg}(t)$.

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Dielectric Properties of Ternary $0.5Y_{0.1}Zr_{0.9}O_2 – 0.5(0.6SrTiO_3 – 0.4BiScO_3)$ Ceramic System

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Ternary $0.5Y_{0.1}Zr_{0.9}O_2 – 0.5(0.6SrTiO_3 – 0.4BiScO_3)$ system should be considered as consisting of two individual subsystems. First of them is zirconium dioxide, ZrO_2, stabilized by Y, so that nominal composition of this subsystem is corresponding to $Y_{0.1}Zr_{0.9}O_2$. Second subsystem is two-component $SrTiO_3 – BiScO_3$ system with a ration of end members corresponding to the $0.6SrTiO_3 – 0.4BiScO_3$ composition. Ternary $0.5Y_{0.1}Zr_{0.9}O_2 – 0.5(0.6SrTiO_3 – 0.4BiScO_3)$ system is attractive to be studied in details due to both interesting properties of the individual subsystems and a change in these properties via combination of the subsystems in a single system [1, 2].

During the preparation of materials based on ternary $0.5Y_{0.1}Zr_{0.9}O_2 – 0.5(0.6SrTiO_3 – 0.4BiScO_3)$ system, an interaction between separate subsystems can take place resulting in deviation of real chemical composition of the subsystems from nominal one and, hence, in changes of their both microstructure and properties. The dielectric properties of solids are sensitive to change of their microstructure and composition. So, the aim of present work is to find and analyse the peculiarities in the dielectric properties of ternary $0.5Y_{0.1}Zr_{0.9}O_2 – 0.5(0.6SrTiO_3 – 0.4BiScO_3)$ ceramic system, in which interaction between the individual $Y_{0.1}Zr_{0.9}O_2$ and $SrTiO_3 – BiScO_3$ is expected. To underline the peculiarities characteristic of ternary $0.5Y_{0.1}Zr_{0.9}O_2 – 0.5(0.6SrTiO_3 – 0.4BiScO_3)$ system, the dielectric properties of this system will be compared to that of two-component $0.6SrTiO_3 – 0.4BiScO_3$ system.

Ceramics samples of the ternary $0.5Y_{0.1}Zr_{0.9}O_2 – 0.5(0.6SrTiO_3 – 0.4BiScO_3)$ system were for the first time synthesized using solid-state processing techniques. XRD analysis shows that the tetragonal $P42/nmc$ phase characteristic of the $5Y_{0.1}Zr_{0.9}O_2$ subsystem and the cubic $Pm\bar{3}m$ and tetragonal $P4mm$ phases characteristic of the $0.6SrTiO_3 – 0.4BiScO_3$ subsystem are coexisting at room temperature. Two various individual subsystems can be also seen by the SEM experiments.

Anomalous changes of the dielectric properties were observed within three temperature fields. The dielectric anomalies corresponding to the lowest temperature field (below room temperature) are associated with the diffuse ferroelectric phase transition. These anomalies are resulted from appearance and temperature evolution of a polar phase distributed inside a nonpolar matrix. Mean temperature dielectric anomalies are corresponding to a dielectric relaxation process with the activation energy of 1.25 eV. The temperature position of these anomalies strongly depends on a measuring frequency and falls in the temperature 600÷900 K range. High temperature dielectric anomalies induced an ionic conductivity are observed above ~900 K. The activation energy of the ionic conductivity was estimated as ~ 2 eV.

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Modeling the Response of a Natural Heterostructure to the Impact of a Pulsed Magnetic Field (PMF)

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Biocomposites of natural origin are able to change their mechanical properties under the influence of external physical factors (ultrasound, pulsed magnetic field (PMF), inhomogeneous temperature field, radiation) [1]. This is due to the influence of factors on the mobility (fluctuations) of the structure of the composites. The result of the response of multicomponent systems to the effect of physical factors is often the formation of chemical bonds between free radicals of macromolecules. If we denote by the parameter η the rate of increase in the fraction of pulses of PMF stimulating the formation of chemical bonds:

$$\eta = \frac{dn}{ndt}, \qquad (1),$$

then for the number of chemical bonds undergoing a change, we obtain a differential equation of the first order

$$\frac{dn}{dt} = \eta n \qquad (2)$$

$$\eta = \eta_0 - \kappa n, \qquad (3)$$

with the initial conditions n = n_0 for t = 0, where n_0 is characterized by the initial number of formed bonds at a fixed value of the pulse amplitude. Existing ideas about the mechanisms of the change in the structure of composite indicate a decrease in the speed η with an increase in the number of bonds formed (this confirms the threshold nature of the dependence of the hardness of the biocomposite on the number of pulses of the PMF) [2]. Therefore, this parameter will decrease with increasing number of generated pulses in the linear approximation as

$$\eta = \eta_0 - \kappa n, \qquad (3),$$

where η0 and κ are model parameters. Equation (2), taking (3) into account, has an analytic solution

$$\Delta n = \frac{\eta_0 \exp(\eta_0 t)}{A + \kappa \exp(\eta_0 t)}, \qquad (4)$$

where A is determined by the relation $A = \frac{n_0}{\eta_0 - \kappa n_0}$. Relation (3) is the basis for calculation of parameters η_0 и κ by the method of optimizing the mean square deviation of the experimental data from the model dependence[3]. The parameters are characteristics of the response of the complex structure of the composite to the external action. This approach makes it possible to predict the behavior of complex composite materials subjected to processing by various physical factors.

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On One Approach to the Analysis of IR-Spectra of Heterostructures of Natural Origin

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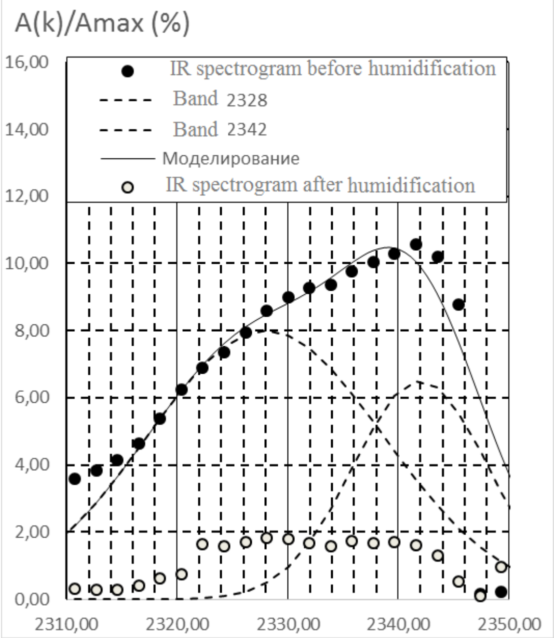

The study of the responses of natural composites to the effects of various physical factors will optimize the methods and modes of their processing to obtain materials with a wide range of physicomechanical characteristics. The properties of heterostructures of natural origin are largely determined by their microstructure, which is distinguished by complexity and irregularity. The method of infrared Fourier transform spectroscopy is optimal for monitoring changes in the microstructure of complex biocomposites, because it promptly studies the majority of vibrational and rotational spectra of molecules [1]. The problem of the wide use of this method in the ambiguity of the interpretation of spectrograms. Spectra of different oscillations overlap, which makes it difficult to unambiguously identify changes in the microstructure. The report proposes to use the method of modeling bands for their unambiguous identification in the case of imposition. The figure shows the IR spectrograms before the wetting of the microtome sections of natural wood (pine) and after, in the region of the typical overlap of two absorption bands (in the figure they are indicated by black and bright dots). The figure shows the IR spectrograms before and after moistening the microtome sections of natural wood (pine), in the region of the typical overlap of two absorption bands (in the figure they are marked with black and white circles). The modeling was carried out by minimizing the root-mean-square deviation of the analytical dependence on experimental data, the profile of each band was modeled by the Gauss function [2]. The results of modeling showed that before and after wetting this part of the spectrogram is the result of the superposition of two bands (2328 cm^{-1} and 2342 cm^{-1}). The decrease in the intensity on this part of the spectrogram after wetting is accompanied by the equalization of the intensity of these bands. Thus, the modeling allows to analyze more subtle changes in the IR spectrograms after exposure to physical factors, which will allow to specify the mechanisms of moisture transfer in the micropores of wood and lead to the ability to obtain materials with certain hydrophobic and dielectric properties.

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Size Effects in the Diisopropylammonium Iodide an Organic Ferroelectric Embedded in an Opal Matrix

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Organic ferroelectrics attract a lot of attention as less hazardous materials than the widespread perovskite barium titanate and lead zirconate titanate. These two ferroelectrics show excellent characteristics, but are limited in their applications due to the presence of heavy metals. Organic ferroelectrics are generally easy and environmentally friendly in processing, have light weight and can be mechanically flexible [1]. They manifest all fundamental properties inherent to non-organic crystalline ferroelectrics; however, can possess special features due to the van der Waals interaction.

In recent years, a number of organic compounds with a polar point group at room temperature and a relatively high melting point (~450 K) have been discovered. Such ferroelectrics include: diisopropylammonium chloride ($C_6H_{16}ClN$), abbreviated DIPAC P_s ~8.2 μC×cm^{-2}, $T_c = 440$ K [2]; diisopropylammonium bromide ($C_6H_{16}BrN$), abbreviated DIPAB P_s ~23 μC×cm^{-2}, $T_c = 426$ K [3]; diisopropylammonium iodide ($C_6H_{16}IN$), abbreviated DIPAI P_s ~33 μC×cm^{-2}, $T_c = 415$ K [4]. In this paper, we present the results of an investigation of the linear and nonlinear dielectric properties of nanocomposites based on opal matrices filled with DIPAI.

At room temperature, DIPAI belongs to the orthorhombic nonpolar chiral spatial group $P2_12_12_1$. However, when heated, depending on the technology of production, two scenarios are possible. In the first case, according to Ref. 4, upon heating to 369 K, a polar monoclinic phase with $P2_1$ symmetry arises, stable to 415 K. Above 415 K, DIPAI passes into the nonpolar monoclinic phase $P2_1/m$. During the cooling process at 407 K, a single phase transition is observed where DIPAI is converted directly from $P2_1/m$ into a polar monoclinic phase with $P2_1$ symmetry. And it remains in this state up to room temperature. According to the second scenario, when the sample was heated to a temperature of 376 K, a phase transition was observed from the nonpolar orthorhombic phase $P2_12_12_1$ to the nonpolar monoclinic phase $P2_1/m$ [5].

Thus, from the temperature dependence of the linear dielectric properties and the amplitude of the third harmonic $\gamma_{3\omega}$, it can be concluded that for the $C_6H_{16}IN$ embedded in the opal matrix, when heated in a temperature range of 362-377 K, a ferroelectric phase arises that is not found in bulk samples. A small change in the temperature of phase transitions is probably related to the relatively large size of DIPAI inclusions in opals, in which the size effect is poorly manifested.

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Size Effects in the LiCsSO_4 Ferroelastic

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Ferroelectrics and ferroelastics are functional materials with broad area of applications. Their spontaneous polarization or spontaneous strain can be switched over by an electric field or mechanical stress that makes them attractive for developing memory cell, various sensors and actuators. At present, studies and fabrication of nanocomposites with ferroelectric and ferroelastic properties are in the focus of solid state physics [1,2]. A method of producing such nanocomposites consists in embedding fine ferroelectric or ferroelastic particles into porous templates. Sizes and arrangements of confined nanoparticles are specified by geometry of the pore network which allows us to create arrays of particles with particular dimensions and interparticle distances. For many nanocomposites with ferroelectric nanoparticles the temperature of the ferroelectric phase transition was found to shift compared to that in the bulk counterparts (see [1,2] and references therein). In the present paper we report results of studies of the change of the ferroelastic phase transition features for the $LiCsSO_4$ particles confined to a porous alumina film. The measurements were carried out by linear and non-linear methods of dielectric spectroscopy.

The $LiCsSO_4$ crystals have an orthorhombic symmetry *mmm* at room temperature. Near 202 K they have the pseudoproper ferroelastic phase transition into a monoclinic symmetry 2/*m* without changes in the number of atoms in the unit cell [3,4].

To get the nanocomposites, we used the porous Al_2O_3 films produced by TopMembranes Technology. The mean pore diameter was equal to 100 nm and the pore period was 125 nm. The pore length was about 50 μm.

The double lithium cesium sulphate was introduced into pores from a warmed LiCsSO4 aqueous solution. Then the film was slowly cooled down to room temperature that initiated the crystallization of LiCsSO4 seeds and subsequent growth of nanocrystals during several days. Then the procedure was repeated twice times more. As a result the LiCsSO4 nanorods were formed within alumina pores. The film was dried under vacuum to remove the excess water. The pore filling estimated by weighing the film was near 60%.

Temperature dependences of the linear permittivity ε' and coefficient of the third harmonic generation γ_3 were studied for the nanocomposite produced by embedding the $LiCsSO_4$ ferroelastic into porous alumina with a pore size of 100 nm compared to the bulk counterpart. The thermal hysteresis was found for the non-linear coefficient γ_3 in the nanocomposite at the ferroelastic phase transition. The phase transition temperature in the nanocomposite increased by 15 K upon warming. The results observed were ascribed to mechanical stresses in confined $LiCsSO_4$ nanorodes.

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The Dielectric Properties of the Nanocomposite Silicon Oxide - Water

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Usually, to obtain composites with water-soluble crystals, the nanoporous matrix is lowered into a solution saturated at a certain temperature and crystals are grown by evaporation in nanochannels. In the pores above the crystals, air nano-regions remain that can be filled with water molecules from the environment. This leads to a large influence of humidity on the properties of such nanocomposites [1].

This paper presents the results of a study of the dielectric properties of a kind of composite amorphous nanoporous silica with water. In this case, the nanoporous matrix was obtained from a nano-dispersed SiO_2 silica hydrosol using the procedure described in [1]. The filling SiO_2 with water occurred from the ambient air, the humidity of which was set by silica gel, which was in the glass together with the sample.

For an annealed sample of pure SiO_2 heated to 120 ^{0}C, the values of the dielectric constant (ε) are small and do not exceed 10. In Fig. 1 shows the characteristic temperature dependence of ε for four successive heating and cooling cycles. The values of ε are rather large, even in comparison with ferroelectrics.

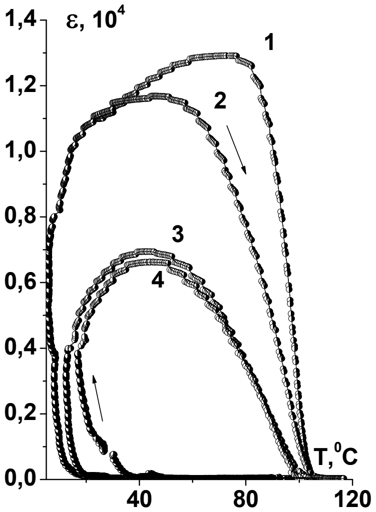

Fig.1.Temperature dependence of SiO_2 composite with water molecules at four continuous heating-cooling cycles. f =1Hz, E= 5V / cm

With a gradual increase in the humidity of the ambient air during heating, the values of ε also increase over the entire temperature range. At a frequency of 0.1 kHz, the dielectric constant is of the order of 10^5.

Despite the large dipole moment of individual water molecules, under normal conditions, the dielectric constant of water is 81.

The large ε of the composite obtained in our studies is silicon dioxide — water can be associated with the specific behavior of water in SiO_2 nanopores. It is assumed that orientational ordering of the dipole moments of individual water molecules occurs in the nanopores of the core, which leads to an increase in the total dipole moment and, as a consequence, an increase in the dielectric constant. It can be assumed that water becomes a kind of superparaelectric, like the existence of superparamagnetic with decreasing particle size [2]. The observed effect should be considered in the context of the manifestation of the ferroelectric properties of water, the possibility of which is discussed in [3].

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The Dynamic Features of the Coefficients Study in the Expansion of the A_2BX_4 Group Crystals Electric Energy on the Polarization by the Harmonic Analysis Method

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According to the theory of Landau-Devonshire [1,2] in the case of a uniaxial ferroelectric we can expand the free energy W_C in powers of the only one component of the polarization P_C. Using the theory of Landau-Devonshire for quantitative evaluations of the measurement results of the polarization properties of the model crystal unit A_2BX_4 - chlorinate rubidium Rb_2ZnCl_4 is applicable in case if the free energy W_C are expanded in powers of the only one component of the polarization limited to members up to the fourteenth degree [3]. Thus, limiting the members to the fourteenth degree of polarization, we have:

$$W_C=\frac{1}{2}aP_C^2+\frac{1}{4}bP_C^4+\frac{1}{6}cP_C^6+\frac{1}{8}dP_C^8+\frac{1}{10}eP_C^{10}\frac{1}{12}fP_C^{12}+\frac{1}{14}gP_C^{14}-EP_C\,, \tag{1}$$

where a, b, c, d, e, f, g are the coefficients that have a certain physical meaning [4], E is the electric intensity.

It is known that the equilibrium configuration ($d(EP_C)/dP_C=E$) is determined by finding the minimum $W_C(P_C)$. This equation in Landau-Devonshire theory gives an expression for the electric field E as a function of P_C polarization. If we use seven members in the decomposition we have:

$$E=aP_C+bP_C^3+cP_C^5+dP_C^7+eP_C^9+fP_C^{11}+gP_C^{13}\,. \tag{2}$$

In the process of measuring the P_C in the dynamics, for example, using the Sawyer-Tower scheme, it is necessary to consider the dynamic features of the P_C measurement, as $d(EP_C)/dP_C=E+P_C dE/dP_C$.

In [3] the repolarization process of group A_2BX_4 model crystal - rubidium chlorate Rb_2ZnCl_4 under the action of harmonic electric field with amplitude higher than the coercive field intensity was investigated by the harmonic analysis method. The time dependence of the current density $J_X(t)$ that arise in the sample under the harmonic field action which intensity is higher than the coercive field intensity, has a complex periodic form.

In this paper the study of the current density harmonics $J_X(t)$ of A_2BX_4 group crystals series allowed to construct the dependence of the energy W_C and the electric intensity E of the sample unit volume on the polarization P_C that were measured in the dynamics, to determine the values of the coefficients a, b, c, d, e, f and g (expression 1).

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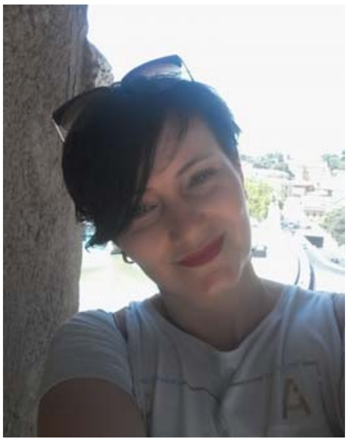
Linear and Non-Linear Dielectric Properties of DTGS in Porous Al_2O_3 Films



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At present, studies of the properties of nanocomposites based on porous matrices with ferroelectric filling are of considerable interest. The physical properties of such structures are affected by effects associated with the size and geometry of the pore grid. As one of the types of such matrices used for the production of nanostructures, is alumina (Al2O3) which is a film with a honeycomb structure of pores, oriented perpendicular to the surface.

In the paper the results of studying linear and nonlinear dielectric properties of nanocomposites based on DTGS, embedded into pourous Al_2O_3 oxide films, are presented. In the experiment Al_2O_3 films were used with the following parameters: the first film had a cell size of 450 nm and a pore diameter of 300 nm, the second film had a cell size of 125 nm and a pore diameter of 100 nm, the pore depth of both films was ~ 50 μm.

The temperature dependences of the dielectric properties and third harmonic coefficient γ3ω of composite materials, obtained by embedding DTGS into porous Al2O3 alumina matrixes with pore diameters of 300 and 100 nm, were studied. The temperature dependences of the effective permittivity and third harmonic coefficient are shown in Fig.1.

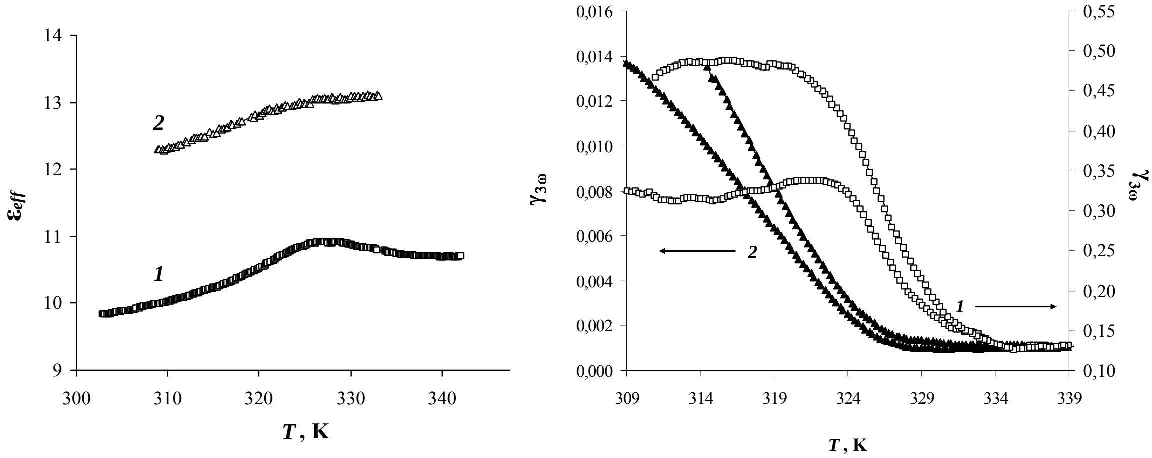

Fig.1. Temperature dependences of the effective permittivity at a frequency of 1 MHz and $\gamma_{3\omega}$ for a samples of DTGS/Al_2O_3 (300 nm) (1) and DTGS/Al_2O_3 sample (100 nm) (2)

As it follows from the experiment, the phase transition is blurred and Curie temperature shifts to low temperature region. A significant decrease in the temperature of the ferroelectric DTGS transition in pores of aluminum oxide may indicate that for DTGS/Al2O3 (100 nm), their own dimensional effects are dominant. Mechanical stresses may not play an important role because of the partial pore filling, and a weak effect of the dipole-dipole interaction is due to the low value of the spontaneous polarization or the disordering of the dipole moments in the pores.

Elastic Properties and Frequency Characteristics of a Novel 3–0-type Three-component Composite

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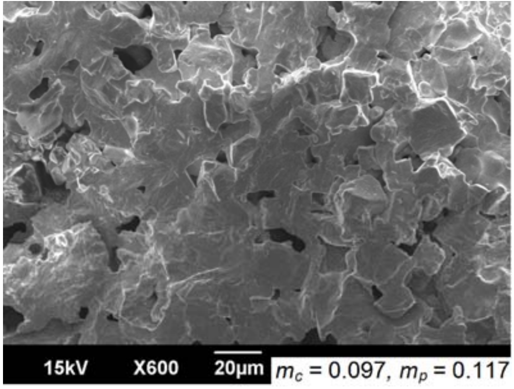
The present study is concerned with a piezo-active composite that contains the ferroelectric PZT-type ceramic, corundum ceramic and air inclusions. The corundum ceramic is a piezo-passive component with a large elastic stiffness in comparison to the stiffness of the ferroelectric ceramic component (ZTS-19 in the composite samples manufactured at ‘Piezopribor’, Institute of High Technologies and Piezotechnics, SFedU), and the volume fraction of corundum is $m_c < 0.2$. Our analysis of micrographs of sections of the composite shows that its microgeometry becomes more complicated on increasing m_c. The composite is characterised as a 3–0–0 material in terms of connectivity [1] where “3” refers to ZTS-19, middle “0” refers to corundum inclusions, and right “0” refers to isolated air pores. Coexistence of the corundum-rich regions (inclusions) and air pores are observed (see the micrograph), and increasing porosity m_p on increasing m_c is stated. We first described the “mirror” behaviour of the volume fractions m_c and m_p in the studied composite at $0.05 < m_c < 0.18$ [2]. The presence of both the corundum inclusions and air pores at their almost equal volume fractions considerably influences the elastic and piezoelectric properties, and this influence is without parallel in composites studied before publishing work [2]. An influence of average sizes of the particles on the performance of the composite is considered.



The studied 3–0-type composite is characterised as a piezoelectric material with relatively stable resonance frequencies at planar (radial) and thickness oscillation modes of samples [2]. Experimental results on the elastic properties and frequency characteristics of the composite are interpreted in terms of a model that takes into account an electromechanical interaction between the 3–0 ferroelectric ceramic / corundum and 3–0 ferroelectric ceramic / pore regions [2]. In the model put forward, the 3–0 connectivity pattern plays the important role in forming the effective electromechanical properties, their anisotropy, acoustic and related parameters of the composite. The composite can be applied as an active element of piezoelectric transducers, sensors etc. where the thickness oscillation mode is dominating.

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Domain Orientations and Piezoelectric Properties in Novel 2–2-type Composites with Two Single-Crystal Components

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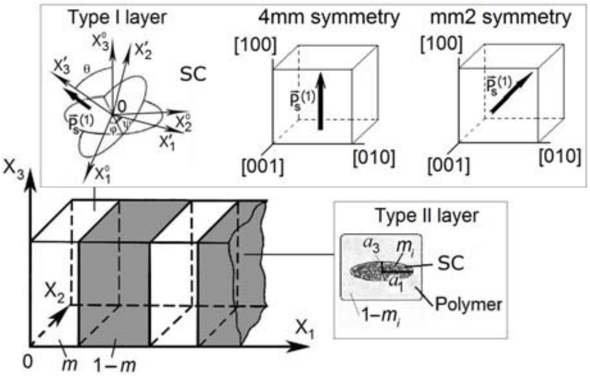
The present report is concerned with the piezoelectric performance and related parameters of the 2–2-type parallel-connected composites. An interest in these materials stems from their piezoelectric performance, hydrostatic parameters [1] and orientation effects [2] at rotations of the main crystallographic axes in ferroelectric single-crystal (SC) components. The composite studied by us consists of layers of two types (Type I and Type II layers, Figure) with interfaces that are parallel to the (X_2OX_3) plane. These layers are regularly arranged along the co-ordinate OX_1 axis. The Type I layer is a ferroelectric single-domain SC, and its spontaneous polarisation is $\boldsymbol{P_s}^{(1)}$. The Type II layer is a SC / polymer medium with 0–3 connectivity. The composite is characterised by 2–0–2 connectivity, and the effective properties are found by means of the effective field method (0–3 connectivity) and matrix method (2–2 connectivity) [2]. Hereby we analyse the role of the domain orientations in the Type I layer in forming the piezoelectric sensitivity (piezoelectric coefficient g_{33}^* and its hydrostatic analog g_h^*) and squared figures of merit $(Q_{33}^*)^2 = d_{33}^* g_{33}^*$ and $(Q_h^*)^2 = d_h^* g_h^*$ of a 2–0–2 PMN–0.37PT SC / $Li_2B_4O_7$ SC / polyethylene composite where d_{33}^* and d_h^* are its piezoelectric coefficients. The piezoelectric properties and related parameters of the 2–0–2 composite depend on the $\boldsymbol{P_s}^{(1)}$ orientation, volume fractions of components and on the aspect ratio of the SC inclusion. We compare data on the related composites: the first is based on the single-domain SC with 4*mm* symmetry, and the second is based on the single-domain SC in the field-induced phase with *mm*2 symmetry. We note the high level of the piezoelectric sensitivity ($g_{33}^* \approx 1$ V·m / N, $g_h^* \approx 1$ V·m / N) and hydrostatic piezoelectric activity ($d_h^* \sim (10^2 - 10^3)$ pC / N) and large values of $(Q_h^*)^2 \sim 10^{-10}$ Pa^{-1} at specific $\boldsymbol{P_s}^{(1)}$ orientations and volume fractions of the PMN–0.37PT SC $m < 0.1$.



Acknowledgment. Research has been carried out at the financial support from the Ministry of Education and Science of the RF within the framework of the complex project “Working out and creation of a high-technological production of a mobile hydroacoustic complex to highlight a situation in various areas of the World ocean on the basis of modern piezoelectric means of the new generation” (contract No. 03.G25.31.0276, May 29th, 2017) by using the equipment of the Centre of Collective Use “High Technologies” at the Southern Federal University.

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V. Domains, Domain Boundaries and their Dynamics

Spontaneous Evolution of the Domain Structure of TGS Crystals

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The kinetics of non-equilibrium domain structure of ferroelectric triglycine sulfate group crystals (pure and doped with L,α-Alanine impurity) has been studied at a short distance from the Curie point ($0.1\ \mathrm{K} \leq \Delta T_C \leq 1.0\ \mathrm{K}$) by means of atomic force microscopy technique (AFM). The domain structure emerged at the phase transition was detected by scanning of the *ac*-surface of a sample in the contact mode of the piezoelectric response using the AFM microscope Solver P47 Pro and cantilevers NSG 11 / TiN.

The regularities of a temporal behavior of the basic parameters of the domain structure (the average size $<w>$ of domains on the *ac*-plane, the total number N and the total perimeter L of domains, the coefficient of static unipolarity φ, the average velocity of the domain walls movement) have been studied in accordance with method reported in [1].

It is shown: 1) the total number of domains N and their total perimeter L decrease exponentially with time; 2) the average sizes of domains along the crystallographic directions [100] and [001] change over time according to the power law $<w> \sim t^{\psi}$. The values of the exponent ψ vary depending on the temperature and equal approximately to 1 in the close proximity to the Curie temperature. It indicates to the evident non-conservativity of the macroscopic order parameter of the domain structures of the studied TGS crystals under conditions of the experiment, and also it shows, that the domain coarsening near the phase transition point can’t be described in the frames of the existing theories of the phase ordering in the systems with scalar order parameter; 3) a noticeable change of the total charge on the *ac*-surfaces of pure and doped TGS crystals was observed only near T_C and approximately during the first 30 minutes after the phase transition, because under these experimental conditions the TGS crystal is an open system with a non-conservative order parameter; 4) the time dependences of the average velocity of the lateral (along [001]) movement of the domain boundaries change qualitatively away from the phase transition temperature.

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Analysis of Model and Real 180^0 Domain Pictures by Means of Space-Time Correlation Functions

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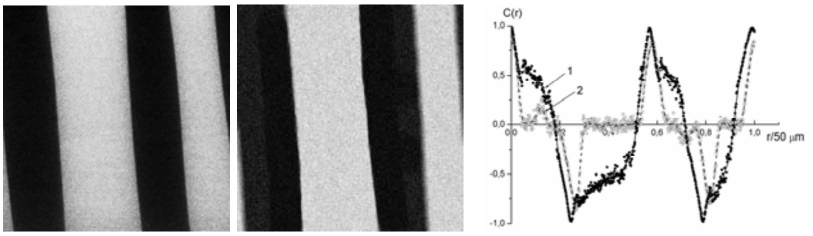
Images of the domain structure, obtained by means of atomic force microscopy technique, with their subsequent mathematical processing can provide essential information about the static and dynamic properties of domains. In particular, the calculation of the equal-time correlation function $C(r,t) = \langle S(r,t)S(0,t)\rangle$, where the scalar order parameter $S(r,t)$ takes the values of +1 and –1, respectively, for r inside domains with opposite directions of the spontaneous polarization, while the brackets denote the spatial average, gave an opportunity to study the ordering dynamics of the observed domain patterns after the quenching of a ferroelectric TGS crystal into the polar phase [1,2]. The set of correlation functions $C\{x=r/L(t)\}=f(x)$, scaled with so called characteristic length $L(t)$, for all the different times over long-term observation of the domain structure evolution of TGS crystal has demonstrated that the scaling hypothesis is satisfied in the present system [3]. Nevertheless, the question is: what is the influence of the quality of the processed domain images in these results?

In the present paper we had made attempt to compare the results of processing of the similar model and real (for TGS crystal) domain patterns. The various domain structures inherent for TGS crystals were simulated and the correlation functions along [001] crystallographic direction were calculated.



a *b* *c*

Fig. Domain images: real for TGS crystal – *a*), simulated – *b*) and their correlation functions *c*): 1 and 2 respectively

As one can see from the Figure, an insignificant difference in the quality of the images (noise, shape of the borders etc.) can considerably influence on the form of the correlation function as well as on the physical conclusions.

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Domain Structure of $Na_{0,5}Bi_{0,5}TiO_3$– $BaTiO_3$ Crystals

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At present the lead-free ferroelectric $Na_{0,5}Bi_{0,5}TiO_3$ (NBT) and NBT-based solid solutions are assumed as promising environmentally friendly materials for piezoelectric applications. The most attractive in practical sense is the system NBT- x% $BaTiO_3$ (NBT-x%BT) with morphotropic phase boundary (MPB), which position has been defined for compositions with x=5-6% BT [1].

The work describes the studies focused on identifying changes in domain structure of NBT crystals with addition of $BaTiO_3$ when approaching the MPB. The crystals of NBT- x% $BaTiO_3$ system (x=0, 3,2%, 5%, 6% in start powder mixture) have been grown by Czhochralski method. Parallel and perpendicular to the growth direction cuts are used for the research. The polarization-optical studies of domain configurations and the light transmission studies on wavelength 632 nm are carried out in temperature range 25^0C-540^0C.

It is known that NBT undergoes the phase transformation from cubic paraphase to tetragonal ferroelastic phase at ~ 540^0C. The rhombohedral phase appears below 200^0C where existence of the spontaneous polarization is indicated. The peculiarity of the temperature behavior of the optical properties of NBT is the presence of the “isotropization” point with hysteresis in temperature range 280-290^{o}C during heating process and at 240^{o}C during cooling process. Visually observed NBT domain structure is usually represented by two states separated by (110)-type walls and is ferroelastic. Orientation of domain walls does not change in the temperature range of 25^0C-540^0C. This is due to the possibility of the existence of walls of the same type in both the rhombohedral and the tetragonal phases. The (100)-type walls typical for the rhombohedral phase are observed only on some samples. Addition of the $BaTiO_3$ leads to significant changes in the domain structure of NBT. So, the perpendicular cuts of NBT-3.2% BT, NBT-5% BT, NBT-6% BT are visually observed as almost monodomain at room temperature. For NBT-3.2% BT, the tetragonal phase is realized in 250-400^0C temperature range, where wedges occur along the (110) direction. The regular zones separated by the (100)-type walls appear in the parallel cuts of the test samples. For both NBT-5% BT and NBT-6% BT cuts almost isotropic state is realized above ~ 180^0C and ~ 200^0C, respectively. This does not contradict the conception of the MPB position between the rhombohedral and tetragonal phases for compositions with x = 5-6% BT. The anomalies in the light transmission temperature dependence correspond to the peculiarities of the temperature behavior of the domain structure. It was found that with an increase of the $BaTiO_3$ content special NBT characteristic temperature regions are shifted. Thus, for NBT-3.2%BT the "isotropization" point is recorded at ~250^{o}C, and the phase transition to the cubic phase occurs near 400^0C. How the $BaTiO_3$ add-ons affect both the formation of the domain structure and the peculiarities of the optical properties is discussed within the framework of ideas about changes in the disordering of the ions which are in the A-site of the NBT crystal lattice.

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VI. Multiferroics

Superparamagnetic Properties in Hole Doped Manganites

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Already 40 years ago, Nagaev [1] studied the inhomogeneous ferro-antiferromagnetic state in magnetic semiconductors and introduced the concept of *ferrons*, *i.e.* magnetic polarons, which are ferromagnetic droplets with a size of about 1-2 nm, arising in an antiferromagnetic semiconductor due to localization of charge carriers introduced by doping the semiconductor. Based on these ideas Kugel *et al.* [2] explain the transport and magnetic properties of manganites of various compositions assuming the existence of ferromagnetically correlated regions in the paramagnetic phase. According to their estimates, the size of ferromagnetically correlated regions (FM droplets) is about 30 Å. Electron spin resonance (ESR) turned out to be very sensitive to the formation of ferromagnetic regions in the paramagnetic phase, as has been reported e.g. for La1-*x*Sr*x*MnO3 in the regime $0.075 \leq x \leq 0.175$, where weak, strongly anisotropic ferromagnetic resonance (FMR) lines appear besides the paramagnetic resonance line at $g \approx 2$ already below 270 K far above the magnetic ordering temperature [3]. The ESR linewidth, which reflects the spin-spin relaxation rate, usually exhibits a critical broadening on approaching magnetic order. Following Raikher and Stepanov, [4] who investigated the FMR in a suspension of single domain particles, we assume that ferromagnetically correlated regions in the paramagnetic phase should have a similar effect on the paramagnetic resonance spectrum like superparamagnetic particles. The authors [4] obtained expressions for inhomogeneous contributions to the width of the line of an ensemble of superparamagnetic particles with uniaxial anisotropy: ΔH=ΔH(1)+ΔH(2)

$$\Delta H(1) = \frac{2\alpha}{\sqrt{3}} H_0 \frac{(\xi_0 - L_1)}{\xi_0 L_1}; \Delta H(2) = 3\sigma H_0 \frac{\xi_0 - 3L_1}{\xi_0^2 L_1}, \text{where } \xi_0 = \frac{\mu H_0}{k_B T},$$

$L_1 = \coth \xi_0 - 1/\xi_0$ - the Langevin function, α - is the damping parameter in the Landau-Lifshitz equation, $\sigma = \frac{W_A}{k_B T}$, W_A - is the anisotropy energy of a superparamagnetic particle.

The parameters of nanoclusters were obtained from complex analysis of the temperature dependences of position and linewidth. To check our assumption, we systematically investigated the zinc-doped lanthanum-strontium/barium manganite La1-*xMex*Mn1-*y*Zn*y*O3 by means of ESR and magnetization measurements. The average size of ferromagnetically correlated regions in the ceramic manganites La1-*x*Me*x*Mn1-*y*Zn*y*O3, *Me* = (Sr, Ba) may reach the values about of 1-2 nm, $\mu \sim 170\mu_B$ and $H_A \sim 230$ Oe.

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Dielectric Properties and Polar State of $PbCo_{1/3}Nb_{2/3}O_3$ Single Crystals

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$PbCo_{1/3}Nb_{2/3}O_3$ (PCN) crystals belong to the family of complex perovskites AB'B''O_3. This family includes the materials with unique physical properties: ferroelectrics and antiferroelectrics, relaxor-ferroelectrics, and multiferroics. The PCN crystals are characterized by a diffuse maximum in the dielectric permittivity in the vicinity of 204-250 K and they have antiferromagnetic phase transition at the temperature of $T_N \approx 130$ K [1-4]. It can be considered as a potential relaxor-multiferroic. However, there is a certain scatter of the experimental data on the dielectric properties and polar state investigations. In the case of PCN, one can expect the appearance of false loops of ferroelectric hysteresis due to the nonlinear conductivity in combination with the relatively large dielectric response. To evaluate the temperature dependence of the polar moment, we used the method of Thermally Activated Depolarization (TSD). However, it is necessary to obtain the data on the nature of the dielectric response and the conductivity in order to correctly measure the TSD.

We present the results of a study of the PE-hysteresis loops, the temperature and frequency dependence of the complex dielectric constant and ac-conductivity in the frequency range from 12 Hz to 100 kHz and in the temperature interval 77-400 K. Investigation of the polar state of the crystal was performed by a TSD method according to a standard measurement scheme in two stages: Field Cooling at 50 V (1.1 kV / cm) down to 77 K and Zero Field Heating after Field Cooling with a constant rate 5 K / min with the depolarization current measurement.

As a result, the temperature dependence of the real part of the complex dielectric permittivity shows the frequency-dependent diffuse maxima in ε' in the temperature range 240 - 250 K. A detailed analysis of the P-E loops reveals the combination of the nonlinear conductivity and the linear capacitance of the samples. The conductivity activation energy is estimated to be 0.43 eV. The investigation of the TSD current shows that the polarization moment decreases nonmonotonically with increasing temperature and it disappears in the vicinity of 215 K. Near 180-200 K there are the two depolarization maxima associated with a complex polar moment.

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Electric Polarization Induced by Phase Separation in Magnetically Ordered and Paramagnetic States of RMn_2O_5 (R=Gd,Bi).

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The electric polarization hysteresis loops and remanent polarization were revealed in multiferroics RMn_2O_5 (R=Gd, Bi) at wide temperature interval (5K - 330K) [1]. The long-range ferroelectric order having an exchange-striction magnetic nature had been observed at low temperatures ($T \leq T_C$ = 30 – 35 K). Along with this, an electrical polarization of a different nature had been found at temperatures $T >> T_C$. A generally accepted point of view is that RMn_2O_5 has sp.gr. *Pbam* (at room temperature). We believe that the high-temperature polarization we observed was caused by the frozen superparaelectric state, which was formed by the restricted polar domains resulting from phase separation and charge carriers self-organization. Charge ordering in RMn_2O_5 and the e_g electron transfer between Mn3+ -Mn4+ ion pairs are key factors responsible for polar electric states of these multiferroics at all temperatures. The double exchange between Mn^{3+}-Mn^{4+} ions induces the phase separation in RMn_2O_5 which is similar to phase separation in $LnAMnO_3$ (A – Sr, Ba, Ca) manganites containing Mn^{3+} and Mn^{4+} ions as well. Phase separation exists at all temperatures and makes the formation of local conductive domains containing Mn^{3+} - Mn^{4+} ion pairs with ferromagnetically oriented spins energetically favorable. The phase separation domains are located in a dielectric antiferromagnetic (paramagnetic) matrix of the original crystal.

Theoretically, the frozen superparaelectric state was considered in the system of isolated ferroelectric nanoscale domains in a dielectric matrix [2]. In this state, hysteresis loops and remanent polarizations are observed. The frozen superparaelectric state turns into the conventional superparaelectric one near T* (T*=100 – 330 K), in which the hysteresis loops are destroyed. The T* values correspond to the temperatures at which the potential barriers of the restricted polar domain reorientations become equal to the kinetic energy of the itinerant electrons (leakage). The application of magnetic field H increases the barriers at the phase separation domain boundaries due to the double exchange growth, thus increasing the T* temperatures. The electric polarization hysteresis loops were measured using the version of the PUND method presented in [3], which was adapted to studies of the local polar domains. The emergence of the local phase separation domains was confirmed in the high-sensitivity 3-crystal X-ray diffractometer measurements and in the permittivity and conductivity investigations. We revealed correlations between properties of the local phase separation domains and hysteresis loops. It has recently been shown [4] that the RMn_2O_5 symmetry at room temperature is a noncentral symmetry, which means that the electric polarization should be existed at room temperature.

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Magnetoelectric Properties of Multilayer $BiFeO_3/CoFe_2O_4$ Films Derived by Sol-Gel Process

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Multiferroic multilayer nanocomposites have broad prospects for application as materials for development of non-volatile random access memory, various types of sensors, spintronic devices. Bismuth ferrite ($BiFeO_3$) is one of the most widely known and practically used magnetoelectric materials. The ferroelectric and antiferromagnetic ordering of $BiFeO_3$ (BFO) are stable with Curie and Neél temperatures of 1098 and 643 K [1]. To improve its magnetic properties can develop composite nanostructures with spinel ferrite $CoFe_2O_4$ (CFO), that has high coercivity magnetization [2]. Thus, the aim of the study was to study the possibilities of efficient combining of BFO and CFO phases using a sol-gel process.

Samples of multilayer nanocomposites (BFO/CFO) were prepared by sol-gel synthesis with using spin-coating method (5000 rpm for 30 sec) on the Pt ($Pt/TiO_2/SiO_2/Si$) substrate. Each coated layer was dried on a hot plate at 300 °C for 10 min. Then, coated film was rapidly thermally annealed at three different temperatures (700, 725 and 750 °C) for 10 min in air environment. Therefore, the structures containing 14 layers (BFO/CFO) with thickness of each layer about 120 nm were produced. X-ray diffraction patterns of the obtained multilayer nanocomposites demonstrated presence of two separate phases of BFO and CFO, which revealed their composite-like structure.

Measured values of leakage currents density for all prepared structures were less than 10^{-8} A/cm^2 at electric field 90 kV/cm. The resulting structures demonstrated co-existence of ferroelectric remanent polarization and magnetization (P_r =65 μC/cm^2, M_r =102 emu/gr for 700 °C; 51 μC/cm^2 and 47 emu/gr for 750 °C). Thus, values of remnant polarization, coercivity and saturation magnetization values decrease with increasing temperature of annealing.

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First-Principle Calculations of Electronic, Magnetic and Optical Properties of Spinels $MnFe_2O_4$ and $FeMn_2O_4$

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Compounds with a spinel structure with the general formula AB_2O_4 attract the attention of the scientific community in connection with the variety of physical properties that arise in these compounds, depending on the chemical composition and cation ordering [1,2]. One of the promising and interesting is the presence of a magnetoelectric effect in spinels containing magnetic ions in the structure. There are 2 non-equivalent cationic positions in the spinel structure, A and B, which have a tetrahedral and octahedral environment, respectively. As a consequence, the replacement of cations at these positions can lead to changes in the magnetic, electronic, optical, and magnetoelectric properties. In addition, spinel can have, as a normal crystal structure (AB_2O_4), and inverse ($B(AB)O_4$).

In the present work, first-principles calculations of the magnetic, electronic, and optical properties of bulk crystals of $MnFe_2O_4$ and $FeMn_2O_4$ with the structure of normal and inverse spinel were carried out. All calculations were carried out within the density functional theory (DFT+GGA) implemented in the VASP package. The total energies of the various magnetic configurations have been calculated (Table 1) and the ground magnetic state in the investigated compounds has been found, which for both compounds turned out to be ferrimagnetic with the opposite direction of spins on the atoms at positions A and B. The polarization in the ground magnetic state for all the compounds were comparable with experimentally measured values [3]. The electronic and optical properties of compounds have been studied and their relation to the structure and composition of the spinels has been established.

Table 1. Magnetic ordering, full energies of various magnetic configurations and magnetic moments for $MnFe_2O_4$ and $FeMn_2O_4$ compounds with normal spinel structure.

.		E, eV	M, μ_B
$MnFe_2O_4$	Mn(↓↑),Fe(↓↑↓↑)	109,5	3,8(Mn); 3,7(Fe)
	Mn(↓↓),Fe(↑↑↑↑)	110,2	3,5(Mn); 3,8(Fe)
	Mn(↑↑),Fe(↓↑↓↑)	109,3	3,8(Mn); 3,6(Fe)
$FeMn_2O_4$	Fe(↓↑),Mn(↓↑↓↑)	113,73	3,5(Fe); 3,7(Mn)
	Fe(↓↓),Mn(↑↑↑↑)	114,45	3,5(Fe); 3,7(Mn)
	Fe(↓↑),Mn(↑↑↑↓)	113,51	3,5(Fe); 3,7(Mn)

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Influence of Thermal Treatment on Structure and Magnetic Properties of Nanocrystalline $BaTiO_3$

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Influence of thermal treatment on crystalline structure, and magnetic properties of initially cubic nanocrystalline $BaTiO_3$ nanoparticles was studied. Samples in the form of disc were prepared by compacting of barium titanate powder (Sigma-Aldrich, USA). Initial particles of cubic perovskite modification of $BaTiO_3$ had a spherical shape with 100 nm average diameter. Obtained samples were annealed in the electrical resistive furnace at air atmosphere under the following scheme: 700 ^{o}C (1 h.) then 1000 ^{o}C (5 h.) and 1200 ^{o}C (1 h.). After each "high temperature" annealing the series of "low temperature" treatments in H_2 atmosphere (250 C^{o} 90 min and then 350 C^{o} 90 min) were implemented.

The magnetic measurements after each treatment were conducted with using a vibrating sample magnetometer. Measurements were carried out at frequency of measured magnetic field $f = 10^{-4}$ Hz and amplitude $H_A = 10000$ Oe. The error of measured values M does not exceeded 10 %.

The experimental results showed the following:

1. Thermal annealing of $BaTiO_3$ nanoparticles with initially cubic perovskite crystalline lattice at 1000 °C during 5 h leads to the formation of ferroelectric tetragonal phase. It was found that the increase of tetragonal distortions increase simultaneously with the annealing temperature ($c/a \approx 1{,}0085$ and $1{,}00976$ for the samples annealed at 1000 and 1200 ^{o}C respectively.)
2. Heat treatment of $BaTiO_3$ nanoparticles under experimental conditions does not lead to any visible increasing of their sizes. However, this annealing leads to the formation of small crystallites agglomerates.
3. Diamagnetic response in nanostructured $BaTiO_3$ is observed after each cycle of annealing in air. However the ferromagnetic M-H loops are appeared after thermal treatment in hydrogen atmosphere.

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Electronic and Magnetic Properties of Structural Defects in $SrTiO_3$(Co)

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The discovery of a room-temperature ferromagnetism in cobalt-doped anatase TiO_2 has initiated a large number of experimental and theoretical studies of diluted magnetic semiconductors and oxide materials, which are promising for application in spintronics. It was shown that insulating samples of $SrTiO_3$(Co) with Co concentration of 14–40% exhibit the ferromagnetism at 300 K [1,2]. The functional properties of $SrTiO_3$ can be significantly improved if magnetic and dipolar orderings can be realized in it simultaneously, for example, by doping this material with magnetic off-center impurities. The search for such magnetic off-center impurities that can result in the onset of a magnetoelectric interaction [3] is currently an actual problem.

The position of an impurity in a crystal, its local environment, and its interaction with point defects can significantly affect the magnetic and oxidation states of Co (several oxidation states are typical for 3*d* transition metals). In practice, the oxidation and magnetic states can be changed by varying the synthesis conditions. The aim of this work is to use XAFS spectroscopy and first-principles calculations to determine the structure, oxidation and magnetic states of structural defects produced by Co in $SrTiO_3$.

Single-phase samples doped with 2–3% Co and different deviations from stoichiometry were prepared by solid-phase synthesis at 1100–1600°C. For the incorporation of cobalt into the *A* or *B* sites of the perovskite structure, the composition of the samples was deliberately deviated from the stoichiometry towards the excess of Ti or Sr. XAFS spectra were recorded at the KMC-2 station of the BESSY synchrotron radiation source at the Co *K*-edge in fluorescence mode at 300 K.

It is shown that when changing the synthesis conditions, one can noticeably change the ratio of the concentrations of cobalt atoms entering the *A* and *B* sites of the perovskite structure. At annealing temperature of 1600ºC, most of the Co atoms enter the *A* site, are in the +2 oxidation state, and are off-center (displacement of ~1 Å). At annealing temperature of 1100ºC and in samples annealed at 1500–1600ºC with deviation from stoichiometry toward the excess of Sr, cobalt mainly enters the *B* site, is in the +3 oxidation state, and forms a complex with the nearest oxygen vacancy.

The obtained interatomic distances and oxidation states were used in first-principles calculations of properties of different structural defects. The calculations were performed using the ABINIT program in the LDA+*U* approximation on 80-atom cubic supercells. As a result, the structure of defects whose geometry and magnetic properties are in agreement with experimental data were obtained. The electronic structure of these defects is used to predict the optical properties of the doped material.

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VII. Miscellaneous

Relaxation Polarization and Negative Capacity

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Negative electrical capacitance detected in a large number of substances. The mechanisms of its emergence are discussed. Such as filling traps with the subsequent release of charge, plasma-like dispersion, the nonlinearity of the processes of rectification of AC, etc. We propose the appearance of a negative capacitance can be explained by the emergence of relaxation polarization and polarization of the ionic displacement in matter [1]. After applying the electric field, the own ions of the substance are displaced, forming dipoles. An electric field directed against the external field appears between the charges of the dipole. In the local areas of impurity ions placement, the resulting electric field can be inverted with respect to the external field, which will lead to the appearance of ionic thermal polarization, giving a negative contribution to the polarization of the substance. In impedance spectroscopy, equivalent electrical circuit of the substance consists of three parallel connected between the chains: the capacity of C_3 (it describes the polarization of elastic ion shifts) the conductivity of the G_3 (it describes pass-through conductivity), chain R_4-C_4 (she describes the process of relaxation of polarization). The relaxation time is positive, but the capacitance $C_4 <0$. The frequency dependence of the real part of the capacitance begins with a negative plateau in its low-frequency part. As the frequency increases, the capacitance module decreases, then the capacitance becomes positive, and its growth is completed by a high-frequency plateau. The frequency dependence of the imaginary part of the capacitance repeats a similar dependence for the relaxation polarization with a positive capacitance. The circular diagram for capacitances has a low-frequency part on the left. There are deviations from the semicircles on the left, associated with the influence of through-conduction. A characteristic feature of the dielectric spectrum of a sample of a substance with relaxation polarization, which gives a negative capacitance, is the appearance of a minimum in the negative area of the frequency dependence of the imaginary part of the complex electrical conductivity. The dielectric loss tangent consists of two components, determined by the contributions of through conductivity and relaxation polarization. A maximum is observed in the frequency dependence of the first part of the same frequency at which the minimum is observed for the imaginary part of the complex electrical conductivity. Can be observed minima in the negative area of the frequency dependence of the imaginary part of the dielectric module and the imaginary part of the impedance with a certain ratio of the parameters of the substance. The described dielectric spectrum is observed in composites based on aluminum oxide in silicone oil [2] and some other substances.

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Impedance Spectroscopy and Processes Electromigration in a Substance

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When an electric field is applied to a sample of a substance, electromigration processes begin in it. In the first approximation, the electromigration processes can be divided into pass-through conductivity, fast polarization processes and relaxation polarization processes. Electromigration processes can be described via impedance spectroscopy. In order to describe each processes of the electromigration, an equivalent electric circuit is selected whose frequency dependence of the electrical impedance characteristics is close to the frequency response of a sample of a substance. In this case, the electrical behavior of the substance can be described both by means of a complex specific electrical conductivity and by means of a complex dielectric constant. In the method of impedance spectroscopy use such characteristics as the tangent of the dielectric loss angle $tg\ \delta$, the tangent of the phase angle between current and voltage $tg\ \varphi\ (\delta + \varphi = \pi / 2)$, complex electrical conductivity, dielectric permittivity, impedance, electrical module. All these physical quantities are used in the method of impedance spectroscopy as quantities that allow finding the correspondence between the electrical response of a substance and the equivalent electrical circuit. A resistor corresponds to pass-through conductivity, a capacitor is used to describe fast polarization processes, sequential R-C chain corresponds to relaxation polarization. It is rare only one type of electromigration develops in a substance. Using the principle of superposition of currents, it is possible to describe the processes of electromigration developing in a substance. To do so, the equivalent circuit must be transformed using parallel connection of the elements responsible for each of the additional types of electromigration. The impedance characteristics change. For each of the combinations of types of electromigration, the frequency behavior of the impedance characteristics was calculated. A table has been compiled to track these changes. Can track the changes that occur, for example, by the frequency dependence of $tg\ \delta$. If only relaxation polarization develops in a substance, $tg\ \delta$ is smooth. If there is also pass-through conductivity, the function has a minimum. And if relaxation polarization is combined with fast polarization processes, there is maximum. The presence of all types of electromigration is described by a function with two extrema, a maximum and a minimum. The development of relaxation polarization always leads to a decrease in **ε'** as the frequency grows, but this drop not unlimited with the simultaneous development of fast polarization processes. [1].

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Modeling of the Structure of Ferroelectric Polymer Systems Using the Synthesis of Discrete and Continual Approaches

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Most of the existing models of ferroelectric polymer systems have several disadvantages. Some of them are based on the continual approach, however, the properties of polymers cannot be described using only the equations of continuum mechanics. [1]. At the same time, the existing discrete models do not take into account the kinematic connection of chain segments [2]. Therefore, it is impossible to investigate in them the effect of chain size and molar mass distribution on the properties of the ferroelectric system.

In this paper, a new model of a ferroelectric polymer system is proposed, which is a synthesis of various models of a polymer system and a low-molecular ferroelectric. The conformations of macromolecules were calculated by the molecular dynamics method in the framework of the Hurst-Harris model, in which the chain has thermodynamic bending rigidity. It is assumed that the chain moves inside the tube (the continuum model of reptations of the Doi), the transverse dimensions of which are self-consistently determined by simulating the arrangement of polar groups by the Monte Carlo method. At the same time, the possible orientations of the polar groups are determined by the average elongation of the chain, since they are rigidly connected to the main chain (the backbone of the macromolecule). The paper presents a method for solving the problem of self-consistency.

The temperature dependences of the intermolecular distances, the parameters of the dipole and quadrupole order, and the heat capacity for various values of the parameters of the interactions and the length of the polymer chain are presented. It is shown that the arrangement of macromolecules in a ferroelectric polymer has a layered character. The conditions are given under which there are two structural transitions in the system.

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The Absorption of Terahertz Electro-Magnetic Waves in Ternary Non-Linear Optical Crystal $CdSiP_2$

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The widest variety of vivid physical effects of both quantum and classical interpretation is studied in the terahertz (THz) frequency range (10^{11}–10^{13} Hz). Due to the constant increase of research objectives in the THz frequency range the task of creating and improving the active and passive elements such as sources of THz radiation is highly relevant. The conversion of IR laser radiation in nonlinear optical crystals is one of the promising methods of generating monochromatic and/or broadband THz radiation.

Application of ternary non-linear crystals such as $ZnGeP_2$ allowed to generate radiation of difference-frequency in the range of 2.7–2.94 THz [1], and to receive broadband radiation in the range of 0.1–3 THz, exciting by femtosecond laser pulses [2]. Non-linear crystal $CdSiP_2$ has advanced optical and physical properties [3], [4], being useful for the effective nonlinear-optical conversion of high-power laser radiation and the generation of THz radiation.

The aims of this work are: to study the $CdSiP_2$ dielectric response in the wide THz-infrared frequency range and to determine the main parameters affecting the effectiveness of crystal's use as a radiation generator in the THz region.

Experimental data were collected in a wide frequency range by methods of backward-wave oscillator, time-domain and infrared spectroscopy. The frequency dependences of the refractive index along the main crystallographic directions of $CdSiP_2$ in the THz–IR region have been derived (Fig. 1). Factorized four-parameter semi-quantum model [5] and model of harmonic oscillator were used for spectra fitting over measured spectral range. The spectra of complex permittivity $\varepsilon^*(\nu) = \varepsilon'(\nu) + i\varepsilon''(\nu)$ and absorption coefficient $\alpha(\nu)$ have been determined. As well, contributions of active optical phonons and additional processes to the total losses are obtained. In our opinion, the contribution of additional absorption is formed mainly by difference multi-phonon processes.

Based on the results of our research we can conclude that single crystal $CdSiP_2$ due to the nature of its dielectric response function has an obvious practical interest for the purposes of non-linear optics.

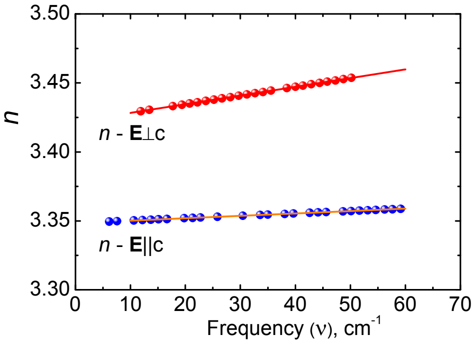

Figure 1. Refraction indexes of $CdSiP_2$ in the THz frequency range.

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Modeling of Physical-Mechanical Processes in Wave Solid-State Gyroscope with Piezoelectric Transducers

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Wave solid-state gyroscopes (WSG) are promising devices for navigation equipment that do not have rotating parts, have durability, small weight and size parameters and power consumption, and are not sensitive to vibrations and overloads [1]. Their accuracy is determined by the optimal choice of the design of the sensing element, the possibilities of its manufacturing technology and electronics. It is important to note that the effectiveness of mathematical modeling depends on the completeness of the mathematical model of the WSG, the chosen numerical method and the capabilities of computing equipment. Mathematical models of WSG, built on the basis of the theory of elasticity of thin axisymmetric shells, quite well describe the behavior of a hemispherical WSG and allow using analytical methods to study the effect of mass and shape defects on its parameters and characteristics, as well as develop algorithms for its balancing [2]. However, in the case of a cylindrical WSG with a more complex form of the suspension of the resonator using piezoelectric transducers for the buildup and removal of the signal, analytical methods lose their effectiveness. The numerical analysis of mathematical models of WSG is required. Thus, in [3], the shapes and frequencies of natural oscillations of cylindrical WSG resonators, as well as thermoelastic losses in them, were calculated using the finite element method.

The physicomechanical processes in the WSG can be adequately described in terms of electrothermomechanics of viscoelastic piezoelectric bodies [4], by introducing volume inertial forces due to the rotation and vibrations of the object on which the WSG is mounted.

In the present report, a mixed boundary-value problem of electrothermal elasticity is formulated and solved numerically for the excitation of resonator oscillations by the piezoelectric elements in the form of thin plates located on it. The shapes and frequencies of the natural modes of the resonator and the influence on them of variations in the sizes of piezoelements are determined. The requirements for thermomechanical stability of the used PZT piezoceramics are established. The factors affecting the good quality of the resonator are considered.

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Solid Phase Transformations in Multilayer Structures Composite – Wide-Gap Semiconductor

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Solid-phase synthesis in multilayer films of nanometer thickness is relevant for electronics materials as a possible way to obtain new metastable compounds, in which a decrease in the temperature of phase transitions is observed. Two systems were considered in the present work: the both systems contain one layer from a $(Co_{40}Fe_{40}B_{20})_{34}(SiO_2)_{66}$ composite, which has superparamagnetic ordering up to the percolation threshold, and the second layer is a gas-sensitive wide-gap semiconductor ZnO (one system) or SnO_2 (another system).

The $[(Co_{40}Fe_{40}B_{20})_{34}(SiO_2)_{66}/ZnO]_{112}$ and $[(Co_{40}Fe_{40}B_{20})_{34}(SiO_2)_{66}/SnO_2]_{32}$ films were obtained by ion-beam sputtering of two different targets. The sputtered material was deposited on the rotating silicon substrates consistently, so as to obtain the multilayer structure where composite and semiconductor (with thickness of 0.5-3 nm) layers were alternated. The structure of the obtained materials in the initial state and after annealing in the temperature range from 250 °C to 600 °C with a step of 50 °C, with a duration of 30 min (with a residual air pressure of $5 \bullet 10^{-2}$ Pa) was investigated by X-ray diffraction in the Bragg angle range from 1° to 60°. All studied films in the initial state have an X-ray amorphous structure but the periodic oscillations are observed on diffractograms in the small angles region (1-10° in a lowangle reflectometry regime). The angular positions of these lowangle peaks correlate with the calculated thickness of the bilayers. The exceptions were observed in films with layer thicknesses less than 1 nm, for which there layered structure has not been formed.

The crystallization of phases as well as solid-phase chemical reactions was observed in the $[(Co_{40}Fe_{40}B_{20})_{34}(SiO_2)_{66}/ZnO]_{112}$ films during the heat treatment. The observed reactions follow the sequence:

$$\text{amorphous} \xRightarrow{400\ {}^{0}C} CoFe;\ Fe_3O_4 \xRightarrow{450\ {}^{0}C} CoFe;\ Fe_3O_4;\ ZnO \xRightarrow{500\ {}^{0}C} CoFe\ ;Fe_3O_4;\ ZnO \xRightarrow{550\ {}^{0}C}$$

$$\xRightarrow{550\ {}^{0}C} CoFe\ ;Fe_3O_4;\ Co_2FeO_2(BO_3);\ ZnO \xRightarrow{600\ {}^{0}C} Fe_3O_4;\ Co_2FeO_2(BO_3);\ ZnO\ ;Zn_2SiO_4.$$

In the $[(Co_{40}Fe_{40}B_{20})_{34}(SiO_2)_{66}/SnO_2]_{32}$ films the phase transformations follow another sequence:

$$\text{amorphous} \xRightarrow{400^{0}C} Fe_3O_4;Co_2Sn \xRightarrow{450^{0}C} Fe_3O_4;Co_2Sn; \xRightarrow{500^{0}C} Fe_3O_4;Co_2Sn;CoSn;SnO_2 \xRightarrow{550^{0}C}$$

$$\xRightarrow{550^{0}C} Fe_3O_4;Co_2Sn;CoSn;SnO_2 \xRightarrow{600^{0}C} Fe_3O_4;CoSn;SnO_2.$$

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Energy Dissipation of Alternating Magnetic Field in High-Temperature Superconductors with Different Microstructure

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It is known that many high-temperature superconductors have ferroelectric properties. In this case, a detailed study of the crystal structure of superconductors with their superconducting parameters is an urgent task [1, 2]. The results of the study of the effect of micro - and nanostructure of multiphase superconducting cuprates are presented $Bi_{2-x}Pb_xSr_2Ca_nCu_{n+1}O_{2n+6}$ (n=1, 2, 3) on their energy dissipation under the influence of superposition of constant and alternating magnetic fields. The samples had a similar microstructure of thin plate crystals of Bi-2212 and Bi-2223 phases growing in arbitrary directions.

In the experiments, we used samples with low density (4.1 g/cm^3), a small value of the critical current at a temperature of 77 K (J_k≈33кA/m^2) and a large width of the superconducting transition ($\Delta T>5$ K). With the obtained samples, a complex of studies was carried out - temperature dependences were measured: complex magnetic permeability, critical current, second and third harmonics.

As a result of studies of the samples, it was found that the curves of harmonic stresses isolated from the sample response signal to an alternating magnetic field have two maxima, one of which is observed in the temperature range of the superconducting transition. It is shown that the value of this" maximum on the dependence $U_n(T)$ grows in proportion to the square of the amplitude of the alternating magnetic field b^2 and in proportion to the frequency f. It is found that such properties are associated with the crystal structure of the obtained superconductors, namely, the ratio of the mass fraction of the phases Bi-2212 and Bi-2223. At high concentrations of the Bi-2223 phase, the maximum is not observed [3]. It is concluded that the energy dissipation of the alternating magnetic field in multiphase superconductors of Bi-Sr-Ca-Cu-O system, which are in the resistive state, occurs in the system of weak phase bonds Bi-2223. Moreover, the energy dissipation of the alternating magnetic field in the system of weak bonds Bi-2223 is more than 10^3 times higher than the energy dissipation in the crystallites of the Bi-2223 phase. It is shown that the mechanism of energy dissipation of the alternating magnetic field in the temperature region of the superconducting transition is associated with golevye losses of induction currents flowing in the system weak ties-phase Bi-2223, and the magnitude of the dissipation is correlated with the magnitude of the voltage odd harmonics.

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Linear Response Function of a Screw Dislocation Near Structural Phase Transition Point

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The vibrations of a screw dislocation in the vicinity of a structural phase transition are considered. This transition, according to the Landau theory [1], was described by the order parameter η. The presence of dislocations leads to the appearance of an additive $\eta_1(\vec{r},t)$ to the thermodynamically equilibrium value of the order parameter η_s, which depends on the radius vector $\vec{r}$ and time t. Earlier bending vibrations edge and screw dislocations in crystals with a soft mode, arising under the influence of external factors in the works of authors [2-4] are studied. In the present work, in contrast to [4] bending oscillations screw dislocation in the arbitrary slip plane are investigated. In the linear approximation from the dislocation displacement the equation of a screw dislocation bending vibrations is obtain

$$\tilde{f}_\perp(q_z,\,\omega)=\alpha_D^{-1}(q_z,\,\omega)\tilde{u}(q_z,\,\omega)\,,$$

where $\tilde{f}_\perp(\vec{q},\omega)$ and $\tilde{u}(\vec{q},\omega)$ are the Fourier transforms of the Peach-Koehler force projection on the slip plane and the dislocation displacement, $\alpha_D(q_z,\,\omega)$ is the linear response function of the screw dislocation near the structural phase transition point, which is found by formula

$$\alpha_D^{-1}(q_z,\,\omega)=\frac{\mu b^2}{4\pi}\int q_\perp dq_\perp\left\{-\frac{(n_y^2-n_x^2)q_\perp^2-2\,\omega^2/c_t^2}{q^2-\omega^2/c_t^2}+n_y^2-n_x^2+\right.$$
$$\left.+\frac{2(n_x^2-n_y^2)q_\perp^2q_z^2\left(1+2(1+\nu)\mu g^2\eta_s^2\tilde{\chi}\right)}{(1-\nu)(q^2-\omega^2/c_t^2)(q^2-\omega^2/c_l^2)-4(1+\nu)\mu g^2\eta_s^2\tilde{\chi}(q^2-\omega^2/c_t^2)^2}\right\}.$$

Here $\vec{q}$ is the wave vector, $q_\perp=\sqrt{q_x^2+q_y^2}$, ω is the frequency, μ is the shear modulus, $\vec{b}=(0,\,0,\,b)$ is the Burgers vector, $\vec{n}=(n_x,\,n_y,\,0)$ is the unit vector of the normal to the slip plane, c_t and c_l are the velocities of transverse and longitudinal sound waves, ν is the Poisson's ratio, g is the constant striction coefficient, $\tilde{\chi}(\vec{q},\omega)$ is the Fourier transform of the order parameter response function to the hydrostatic pressure.

In the case of natural vibrations of dislocation $\alpha_D^{-1}(q_z,\,\omega)=0$ should be assumed. From this equation, the eigenfrequencies of bending dislocation oscillations in the vicinity of the structural phase transition and their damping, the effect of the interaction of an elastic field with a soft mode on the effective mass and the effective rigidity of a dislocation can be established.

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Linear Response Function of a Mixed Dislocation Near the Structural Phase Transition Point

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Mixed dislocation lying along the axis Oz of the vector tangent to the dislocation line $\vec{\tau}_0 = (0,\ 0,\ -1)$, the Burgers vector $\vec{b} = (b_x,\ 0,\ b_z)$ and the vector normal to the slip plane of the dislocation $\vec{n} = (0,\ 1,\ 0)$ is considered. Small vibrations of the dislocation near the equilibrium position are limited. Earlier bending vibrations edge and screw dislocations in crystals with a soft mode, arising under the influence of external factors in the works of authors [1-3] are studied. Structural phase transition, according to the Landau theory [4], was described by the order parameter η. In the linear approximation from the dislocation displacement the equation of a mixed dislocation bending vibrations is obtain

$$\widetilde{f}_\perp(q_z,\ \omega) = \alpha_D^{-1}(q_z,\ \omega)\widetilde{u}(q_z,\ \omega)\,,$$

where $\widetilde{f}_\perp(\vec{q},\omega)$ and $\widetilde{u}(\vec{q},\omega)$ are the Fourier transforms of the Peach-Koehler force projection on the slip plane and the dislocation displacement, $\alpha_D(q_z,\ \omega)$ is the linear response function of the mixed dislocation near the structural phase transition point, which is found by formula

$$\begin{aligned}\alpha_D^{-1}(q_z,\ \omega) = -\frac{\mu}{2\pi}\int q_\perp dq_\perp \Bigg\{ &\left(\frac{1}{1-\nu} + 2\frac{1+\nu}{1-\nu}\mu g^2 \eta_s \widetilde{\chi}\right) \times \\ &\times \frac{b_x^2 q_\perp^4/4 + b_z^2 q_z^2 q_\perp^2}{\left(q^2 - \omega^2/c_t^2\right)\left(q^2 - \omega^2/c_l^2\right) - 4\mu \frac{1+\nu}{1-\nu} g^2 \eta_s^2 \left(q^2 - \omega^2/c_t^2\right)^2 \widetilde{\chi}} - \\ &-\left(\frac{1}{1-\nu} + 2\frac{1+\nu}{1-\nu}\mu g^2 \eta_s \widetilde{\chi}\Big|_{q_z=0,\omega=0}\right) \frac{b_x^2/4}{1 - 4\mu\frac{1+\nu}{1-\nu} g^2 \eta_s^2 \widetilde{\chi}\Big|_{q_z=0,\omega=0}} + \\ &+ \frac{b_x^2 q_\perp^2/2 + b_z^2 q_z^2 - b^2\omega^2/c_t^2}{q^2 - \omega^2/c_t^2} - b_x^2/2 \Bigg\}.\end{aligned}$$

Here $\vec{q}$ is the wave vector, $q_\perp^2 = q_x^2 + q_y^2$, ω is the frequency, μ is the shear modulus, ν is the Poisson's ratio, g is the constant striction coefficient, η_s is equilibrium value of the order parameter, $\widetilde{\chi}(\vec{q},\omega)$ is the Fourier transform of the order parameter response function to the hydrostatic pressure, c_t and c_l are the velocities of transverse and longitudinal sound waves. In the case of natural vibrations of dislocation $\alpha_D^{-1}(q_z,\ \omega) = 0$ should be assumed.

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Linear Response Function of a Mixed Dislocation in a Ferroelectrics Near the Phase Transition Point

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The small bending vibrations of a mixed dislocation in a ferroelectric crystal near the phase transition point similar to those of edge and screw dislocations [1-4] are investigated. Ferroactive axis coincides with a coordinate axis Oz: $\vec{P} = (0, 0, P)$, along the same axis equilibrium position of the dislocation line: $\vec{\tau}_0 = (0, 0, -1)$ with the Burgers vector $\vec{b} = \left(b_x,\ 0,\ b_z\right)$ is located. Linear response function is found

$$\begin{aligned}
\alpha_D^{-1}(k_z,\,\omega) = {} & \frac{\mu}{2\pi}\int k_\perp dk_\perp \left\{ \frac{\mu}{4}\frac{1+\nu}{1-\nu} P_0^2 g_2 \tilde{\chi} b_x^2 k_\perp^4 \left[(3g_1+g_2)\frac{\omega^2}{c_t^2} - 4g_1 k^2 - 2g_2 k_\perp^2 \right] \times \right. \\
& \times \left(k^2 - \frac{\omega^2}{c_t^2} \right)^{-1} \left(k^2 - \frac{\omega^2}{c_l^2} \right)^{-1} \left[\left(k^2 - \frac{\omega^2}{c_t^2} \right) - \mu g_2 (g_1 - g_2) P_0^2 \tilde{\chi} \left(\frac{2g_1}{g_1 - g_2} k_\perp^2 - \frac{\omega^2}{c_t^2} \right) \right]^{-1} + \\
& + \frac{\mu}{2}\frac{1+\nu}{1-\nu} b_x^2 \frac{P_0^2 \left[g_1^2 - \frac{\nu}{1+\nu} g_2 (g_1 + g_2) \right] \tilde{\chi}\big|_{k_z=0,\,\omega=0}}{1 - 2\mu g_1 g_2 P_0^2 \,\tilde{\chi}\big|_{k_z=0,\,\omega=0}} - \frac{1}{4(1-\nu)} \frac{b_x^2 k_\perp^4 + 4 b_z^2 k_z^2 k_\perp^2}{(k^2 - \omega^2/c_l^2)(k^2 - \omega^2/c_t^2)} + \\
& + \frac{b_x^2}{4(1-\nu)} - \frac{\mu}{2}\frac{1+\nu}{1-\nu} P_0^2 \tilde{\chi} [(g_1+g_2) b_x^2 k_\perp^4 + g_1 b_z^2 k_z^2 k_\perp^2] \left[g_1 \left(k^2 - \frac{\omega^2}{c_t^2} \right) + \frac{g_2}{1+\nu} \left(k_\perp^2 - \frac{\omega^2}{2c_t^2} \right) \right] \times \\
& \times \left(k^2 - 2\frac{\omega^2}{c_t^2} \right)^{-1} \left(k^2 - \frac{\omega^2}{c_l^2} \right)^{-1} \left[\left(k^2 - \frac{\omega^2}{c_t^2} \right) - \mu g_2 (g_1 - g_2) P_0^2 \tilde{\chi} \left(\frac{2g_1}{g_1 - g_2} k_\perp^2 - \frac{\omega^2}{c_t^2} \right) \right]^{-1} + \\
& + \frac{b^2 \omega^2 / c_t^2 - b_x^2 k_z^2 - b_z^2 k_\perp^2 / 2}{(k^2 - \omega^2 / c_t^2)} + \frac{b_z^2}{2} + g_2 P_0 \tilde{\chi} b_x^2 k_\perp^2 \left(k^2 - \frac{\omega^2}{c_t^2} \right)^{-1} \times \\
& \left. \times \left[\left(k^2 - \frac{\omega^2}{c_t^2} \right) - \mu g_2 (g_1 - g_2) P_0^2 \tilde{\chi} \left(\frac{2 g_1 k_\perp^2}{g_1 - g_2} - \frac{\omega^2}{c_t^2} \right) \right]^{-1} - b_x^2 \frac{g_2 P_0 \,\tilde{\chi}\big|_{k_z=0,\,\omega=0}}{k_\perp^2 \left(1 - 2\mu g_1 g_2 P_0^2 \,\tilde{\chi}\big|_{k_z=0,\,\omega=0} \right)} \right\},
\end{aligned}$$

where $\vec{k}$ is the wave vector, $k_\perp^2 = k_x^2 + k_y^2$, ω is oscillation frequency, μ is shear modulus of the crystal, ν is Poisson's ratio, c_t и c_l are the transverse and longitudinal sound velocities, g_1 and g_2 are striction coefficients, $\tilde{\chi}$ is susceptibility of a ferroelectric crystal, P_0 is polarization equilibrium value in a homogeneous crystal.

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The Structure and Electrical Properties Heterogeneous System In_2O_3/SnO_2

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The purpose of the work is the creation of a multilayer system with thickness individual layers of 1-2 nanometers. The films with such thicknesses are affected by the processes of surface and bulk diffusion of atoms both during and after synthesis. In addition, there is the possibility of mutual solubility of the elements of a layered structure and the formation of thermodynamically stable compounds between them.

The experimental samples were obtained by the method of ion-beam sputtering of a composite target (In_2O_3 and SnO_2) on a rotating substrate [1].

The thickness of the films obtained varied from 60 to 390 nm. The number of bilayers was 69.

A comparative analysis of the angular dependences of the X-ray scattering intensity I(2Θ) of pure oxides and a heterogeneous nanosystem showed that the indium oxide in the original state has a crystalline structure. The tin oxide and the system In_2O_3/SnO_2 is amorphous.

A possible explanation for this experimental fact is the formation of a complex compound In-Sn-O in the process of film synthesis.

On the low-angle dependences I(2Θ) of the In_2O_3/SnO_2 system, the presence of peaks was revealed. The calculation of the period of the diffraction grating is consistent with the thickness of the bilayers calculated from the deposition conditions. This allows us to conclude that the In_2O_3/SnO_2 structure is multilayered in the original state.

After heat treatment above 500 °C, the films begin to crystallize with the release of the indium oxide, and the multilayer disappears.

Studies of the thermal stability of the electrical properties of the multilayer In_2O_3/SnO_2 system during heat treatment to 600 °C showed a change in the temperature coefficient sign (from negative to positive) and a decrease in electrical resistivity to 6 orders of magnitude depending on the thicknes of the layers.

This is due to the crystallization of the system under study, leading to the destruction of the multilayer structure of the samples and the formation of fine-level states in the band gap of the semiconductor.

Acknowledgments. This work was supported by the Ministry of Education and Science of the Russian Federation as the project part of the state task (No 3.1867.2017/4.6).

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Effect of Iron Doping on the Properties of $La_{0.5}Sr_{0.5}Mn_{1-y}Fe_yO_3$

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The interest to mixed-valence $R_{1-x}A_xMnO_3$-type manganites (where R is a rare-earth element, A is a divalent alkaline-earth element) arises due to the colossal magnetoresistance effect (CMR effect) which was observed in these compounds (see reviews [1,2]). Ceramic samples $La_{0.5}Sr_{0.5}Mn_{0.9}Fe_{0.1}O_3$ (LSMFO) were prepared using conventional solid phase techniques [3]. Iron doping effect in manganites is also interesting for study because Fe^{3+} ion has the same radius as it Mn^{3+} has, and Fe^{3+} is magnetic but non-Jahn-Teller cation and does not involved into the double exchange. The magnetization and electrical resistivity measurements have been also performed in the temperature range of 20 ÷ 300 K in magnetic fields up to 1 T (Fig.1). According to the research, it was established the temperature ranges (T = 148 ÷ 300 K) Efros-Shklovskii mechanisms of hopping conductivity (Fig.2). Were calculated micro parameters in density of localized states (DOS) for LSMFO samples.

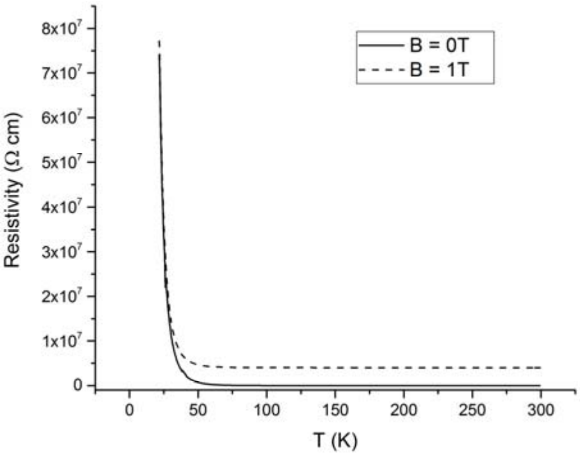

Figure 1. Temperature dependence of the resistivity in the investigated LSMFO samples at B = 0 and B = 1T.

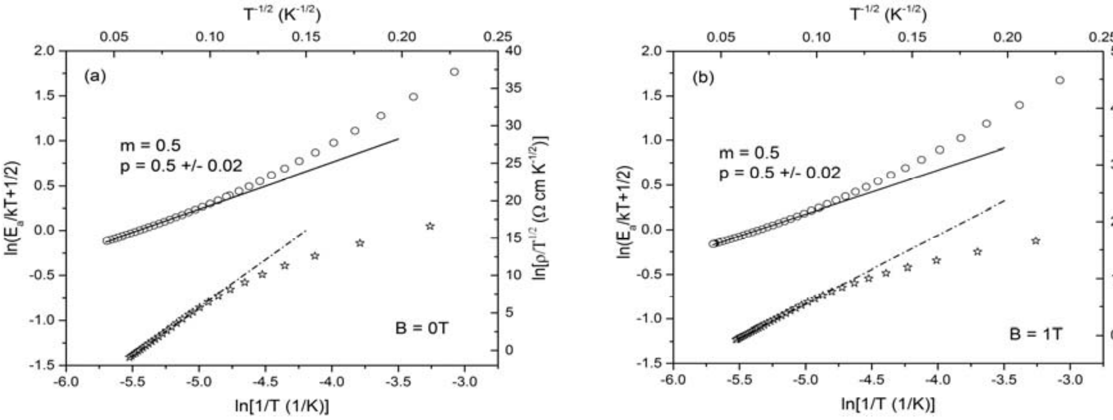

Figure 2. Top panel: the plots of $\ln(\rho/T^{1/2})$ versus $T^{-1/2}$ at $B = 0$ (a) and $B = 1T$ (b) for the temperature intervals HTM (150K < T < 300K). The lines are linear fits. Bottom panel: the plots of $\ln(E_a/kT + m)$ on $\ln(1/T)$ for $m = 1/2$. The lines are linear fits.

Acknowledgment. This work was supported by Russian Foundation for Basic Research (Grant №17-02-00262.)

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Electrical Properties of Ceramic Materials In_2O_3 – ZnO

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Samples of ceramics $(In_2O_3)_{0,33}(ZnO)_{0,66}$ were synthesized by multistage synthesis from powders of zinc oxide and metallic indium. The initial powders was mixed in a ceramic mortar for 90 minutes. The synthesis temperature was sequentially increased to 350, 627, 927 °C in air, the exposure time was 5 hours, then cooling was carried out in the furnace. It is important to note that the process of In_2O_3 solid-phase synthesis from In powder finishing at the temperatures of 627 - 927 °C.

The DC resistivity mesurements of In_2O_3 – ZnO samples were carried out in the temperature range from –196 °C to 150 °C. With treatment temperature increasing from 350 °C to 627 °C, the resistivity of the sample increases too, and the temperature coefficient of resistance (TCR) becomes negative. Annealing of $(In_2O_3)_{0,33}(ZnO)_{0,66}$ samples at a temperature of 927 °C led to complete oxidation of In inclusions. Various results were obtained on control samples: “low” and “high” resistance state. Analysis of the microstructure by X-ray diffraction no revealed significant differences.

The reason for this various sample behavior is apparently related to the fact that areas of zinc oxide contain a small amount of indium. The increase in conductivity in the "low-resistance" sample is realized due to the dissolution of donor impurities. This leads to an increase in the concentration of free charge carriers and an effective decrease in resistance. The samples parameters are demonstrated the best performance in terms of practical application, are presented in table 1.

Table 1

Parameter	Value
Conductivity, σ (resistance, ρ)	125 $Sm \cdot m^{-1}$ (0.008 Ohm·m)
Thermopower coefficient	90 $\mu V / K$
Power factor, PF	1 $\mu W / m \cdot K^2$

According to the literature data, the resistance of annealed zinc oxide samples at T > 1000 [1] monotonically decreases with increasing temperature. However, in some cases [2], the dependence of the conductivity of zinc oxide on temperature is complex at T <450 ºC. This is due to several reasons: the method of synthesis of samples, the rate of heating or cooling (quenching, slow cooling), exposure to air at lower temperatures. By controlling the surface state of the ZnO and In2O3 crystallites, the values of PF and ZT, which are acceptable for practical use, can be achieved at temperatures well below 1000 ° C.

This work was supported by the Ministry of Education and Science in the framework of the project part of the state task (project No. 3.1867.2017 / 4.6).

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The Formalized Simulation of Changes in Polarization of a Linear Pyroelectric in an Inhomogeneous Temperature Field

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Flexible crystallizable polymers exhibit pyroelectric properties and give technological advantages in the manufacture of detectors and radiation receivers of various shapes and geometric sizes. The results of [1] show that the crystallization of polyethylene oxide from a melt in an inhomogeneous temperature field increases the polarization of the samples due to the increase in the size of polar fragments of spherulites forming a crystalline field. The authors of [1] used the method of polarization currents and concluded that the method can be used to observe the kinetics of crystallization of linear polymers. The paper proposes the principles of constructing a formalized model for estimating the parameters characterizing the growth of crystallites in linear polymers in an inhomogeneous temperature field during the melt-crystal transition by means of the experimental dependence of the polarization on the temperature P (T) [1].

Experimental studies show that the magnitude of the change in polarization is directly proportional to the change in the concentration of crystallites [1]. The relative change in the concentration of polymer crystallites dn/n depends on the crystal growth process $\Delta x/x_k$ ($x_k = G/k_D$ is the average crystallite size characterized by the ratio of its growth rate G to the diffusion coefficient k_D of non-crystallizing elements). In the stationary state we can assume that [2]:

$$dn/n = -\Delta x/x_k \ . \tag{1}$$

The thermal expansion of the crystallites occurs by an amount Δx in an inhomogeneous temperature field. Δx is determined by the relation:

$$\Delta x = \alpha x'_k dT \, , \tag{2}$$

where α is the coefficient of thermal expansion, x'_k is the average crystallite size, in the linear approximation it is determined by the relation:

$$x'_k = x_k(\delta - \kappa n) \, , \tag{3}$$

where δ and κ are constants characterizing the kinetics of the formation of crystallites in the polymer. Equation (1) is transformed into a first-order differential equation taking into account (2) and (3):

$$dn/dT = -\alpha(\delta - \kappa n)n \ . \tag{4}$$

The solution of the equation is

$$\Delta P/P_0 = \Delta n/n_0 = \alpha\delta K_{n_0} \exp(-\alpha\delta\Delta T)/(1 + \alpha\kappa K_{n_0} \cdot \exp(-\alpha\delta\Delta T) \, , \tag{5}$$

where ΔT is the absolute value of the temperature inhomogeneity, $K_{n_0} = n_0/\alpha(\delta - \kappa n_0)$ is the normalization coefficient determined by the initial concentration of crystallites n_0. Relation (5) is the formalized model for estimating the ratio κ/δ by the linear regression method using the experimental data *P (T)* for any polymer. For example this parameter is 5% per 1 m^3 for polyethylene oxide.

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Evolution of the Atomic Structure of $Cu_{60}Pd_{40}$ Metallic Glass Under Uniaxial Tension

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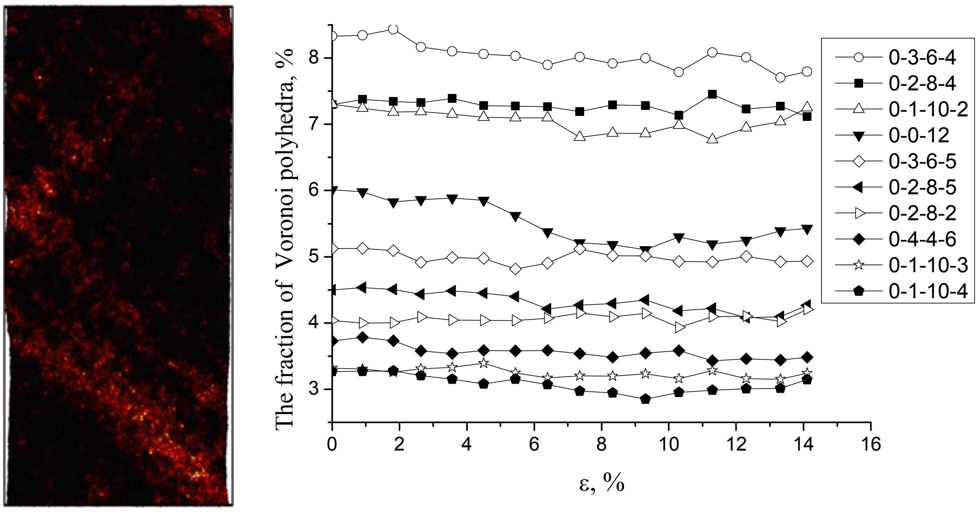
The molecular dynamics method was used to study the laws of the atomic structure rearrangement of metallic glass $Cu_{60}Pd_{40}$ under conditions of uniaxial tension. The computer model contained 500000 atoms, the deformation was carried out at a rate of 6.67×10^{7} c^{-1} while maintaining a constant temperature of 50 K.

In the process of deformation, atomic stresses were calculated [1], the magnitude of quadratic non-affine atomic displacements $D^2_{\min}$ [2], and a statistical and geometric analysis was performed based on Voronoi polyhedra.

It has been established that in the strain interval of 4.5–7.3%, the strain is localized into two narrow shear bands. In Fig. 1, a the image of the model is shown at a deformation of 7.3%, the color of the atoms denotes the value of $D^2_{\min}$ (lighter - more). In the region of shear band propagation, there is a noticeable decrease in the number of Voronoi polyhedra with an index (0–0–12), which correspond to icosahedral coordination polyhedra (Fig. 1, b).



a b

Fig. 1. Image of the model after the termination of the propagation of the shear bands (a) and the dependence of the fraction of different Voronoi polyhedra on the magnitude of the deformation in the shear band region (b)

A model of generation and propagation of shear bands is considered, based on ideas about the formation of an elastic stress field, equivalent to a dislocation field localized in the region of maximum concentration gradient of local centers of shear rearrangements.

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The Pulsed Magnetic Field Influence on Sn Diffusion in α-Fe at 730°C

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Experimentally, it was shown that the pulsed magnetic fields (PMF) have a significant influence on the diffusion mobility of solute atoms in ferromagnetic α-Fe [1,2], and the magnitude of its influence depends generally on magnetization, which is a function of temperature, magnetic field intensity, and the microstructure. In work [1] it was speculated that the magnetic field dependence of Al diffusion in α-Fe is dominated by interactions of the elastic fields caused by solute atoms with the elastic fields induced by moving magnetic domain walls. Later on, a hypothesis about the existence of relaxation mechanisms of the PMF impact on diffusion rates of non-magnetic solutes in α-Fe was put forward [2]. In order to verify the hypotheses, the PMF impact on Sn diffusion in ferromagnetic α-Fe at 730 °C are presently investigated and remarkable changes of the Sn diffusion rates under applied pulsed magnetic field are found.

The frequency dependence of the Sn diffusion rate in α-Fe has a "resonant" character within the frequency range of 1 to 21 Hz and the amplitude intensity of 238.8-398.0 kA/m. The peak value of the Sn diffusion coefficient is larger than that without the magnetic field by a factor of 1.5 to 2.0. At a lower magnetic field of 39.8-79.6 kA/m, the diffusion coefficient does not practically depend on the frequency (within the given frequency range) and the maximum value of the Sn diffusion coefficient in α-Fe is even lower than that in the field-free sample.

The present experimental data suggest that there are two basic mechanisms of the influence of PMF on mobility of a non-magnetic solute in α-Fe, however the "resonant" behavior of the Sn diffusion coefficients indicates strongly the existence of relaxation processes affecting solute diffusion under pulsed magnetic field.

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The Kinematic Origin of Electronic Bound States in Continuum in Planar Semiconductor Heterostructures

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Electronic states are considered with energies within the continuum spectrum but spatially localized in the inner layer of a planar semiconductor heterostructure (PHS). Analogous so called bound states in the continuum (BIC) were found recently in various quantum systems such as semiconductors [1], graphenes [2], quantum Hall insulators [3], optical structures [4].

We present a simple model within single band approximation that demonstrates how electronic states of energies above conduction band edge out of the PHS inner layer and of high enough quasimomenta become confined in the layer due to spatial modulation of effective mass interfered with nonzero band offsets at interfaces of the PHS.

As revealed by the further analysis, the physical origin of the confinement effect is very simple and seems to be not sensitive to details of the theoretical model such as the choice of boundary conditions for envelope wave functions, the validity of the effective-mass or single band approximations and so on. In fact the BIC states in PHS appear to arise due to mere kinematics and to the conservation laws for energy and quasimomentum. Understanding this allows to make definite conclusions on the possibility for the BIC states to exist in a PHS with great band offsets when effective-mass approximation is no longer sufficient to describe details of electron energy spectrum quantitatively.

The kinematic consideration of the over-barrier confinement in PHS gives us a basis to formulate a generalized criterion for the BIC effect. The criterion is valid even for domains of the Brillouin zone quite distant from valleys of the dispersion law when the notion of carrier effective mass is therefore meaningless. Namely, let the bulk dispersion laws in two adjacent layers of the PHS be $E_+(k,k_z)$ and $E_-(k,k_z)$, where k_z is transversal (normal-to-the-plane) component of quasimomentum. Assume further that there exists a domain Ω of E and k values such that of the two equations

$$E_-(k,k_z)=E\ ;\ E_+(k,k_z)=E \tag{1}$$

the first equation has a solution while the second one has not. Then there could appear BIC electron states in the domain Ω. This criterion gives a principal possibility to design structures with unusual properties due to the BIC effect by selecting materials along with their electronic spectra over the whole Brillouin zone for the bulk materials which the PHS is composed of.

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Polarization and Repolarization Processes in Multicomponent Piezoceramics Based on PZT with a Highly Diffuse Phase Transition

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It is known that in the multicomponent ferroelectric ceramic with specific ratio of components of solid solution and modifying additives, the phase transition from ferroelectric phase to paraelectric phase happens in several stages. At the same times, the temperature interval of these structural and polarization changes can reach hundreds degree [1, 2].

In this work repolarization processes and behavior elastic properties in the PZT-based ferroelectric $\left(0.36PbTiO_3 - 0.33PbZrO_3 - Pb(MgZn)_{1/3}Nb_{2/3}O_3 - BaTiO_3 - SrZrO_3\right)$ material are studied.

Figure 1 presents temperature dependence of the effective dielectric constant $\varepsilon'_{eff}=P/\varepsilon_0 E$ and the effective dielectric loses $\varepsilon''_{eff} = \varepsilon'_{eff}\,\mathrm{tg}\delta_{eff}$ (P – the polarization determined by Sawyer-Tower method, E – the amplitude of the measuring field, $\mathrm{tg}\delta_{eff}$ – effective dielectric loss tangent $\left(\mathrm{tg}\delta_{eff} = S/_{\pi EP}\right)$, S – area of polarization loop, measured in the coordinates of digital oscilloscope) in material at frequencies 0.1, 1 and 10Hz in wide range of temperatures of the diffuse phase transaction.

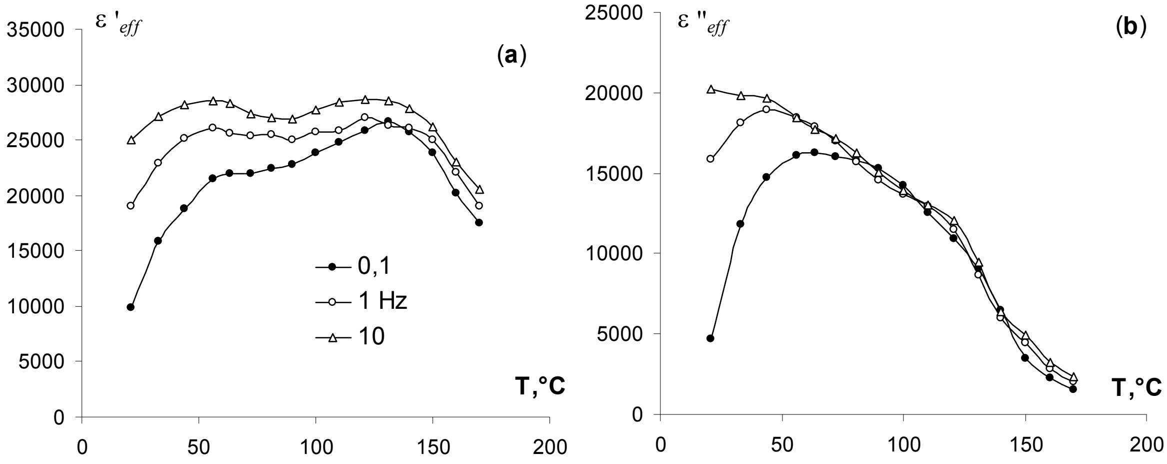

Figure 1 - Temperature-frequency dependence ε'_{eff} - (a) and ε''_{eff} - (b) for a multicomponent piezoceramic material of this composition.

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Evaluation of the Ionizing Radiation Effect on the Viscoelastic Properties of Butyl Rubber Vulcanizates

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In accordance with the classification of polymers by the type of prevailing radiation-chemical transformations, butyl rubber is mainly classified as destructible [1]. The radiation-chemical yield of destruction is directly proportional to the dose of radiation and the molecular weight of the decomposition products. During the processing of rubber based on butyl rubber with ionizing radiation, due to the occurrence of destruction processes, materials with specified plasto-elastic properties can be obtained [2]. Adjustable destruction of polymers can be achieved by establishing patterns and selecting the optimal process conditions in order to obtain the final product with the necessary set of properties.

The aim of the study is to evaluate the effect of ionizing radiation on the viscoelastic properties of butyl rubbers and to create a mathematical description of the radiation destruction process, which allows predicting the viscoelastic properties of the resulting reclaimed rubber. The vulcanizates of butyl rubber, differing in the type of vulcanizing group and fillers, were used as objects of study. The rubbers were irradiated at a Cobalt-60 source with doses of 20-100 kGy.

On the basis of an experimental study of the radiation destruction process of butyl rubber using sol-gel method and viscometry, it was found that the destruction of vulcanizates proceeds mainly along the main polymer chain. It is noted that with increasing dose, an intensive decrease in the Mooney viscosity is observed with a simultaneous decrease in the gel fraction.

A mathematical description of the dependence of the change in the viscoelastic properties of polymer compositions on the irradiation conditions in time is obtained. Using the mathematical model, the dynamics of changes in the concentration of radicals as a function of the absorbed dose was evaluated. It is shown that the rate of viscosity change with an increase in the absorbed dose changes and tends to zero at the passage to the limit. The possibility of determining the required radiation dose to achieve the required viscosity of elastomeric compositions has been established. Using the mathematical model, the kinetic parameters of destruction were evaluated as a function of the radiation dose of butyl rubber vulcanizates. The proposed model of polymer destruction under the action of ionizing radiation of various doses allows to predict their viscoelastic properties.

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Methods for Evaluating of Elastomer's Relaxation Spectrum by Acoustic Spectrometry Data

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One of the methods characterizing the properties of elastomers in a wide range of external mechanical impact frequencies is elastomer relaxation spectrum. It can be obtained using acoustic spectrometry methods. In practice large errors occur at the acoustic information processing for calculating the elastomer relaxation spectrum by numerical methods used to solve such problems. This is due to the fact that they (numerical methods) are based on the calculation of the relaxation spectrum in the frequency range that overlaps the phase transition zone, which is not always possible. In finding the relaxation spectrum by the acoustic spectrometry method, the frequency range is limited by the characteristics of the used ultrasonic transducers [1].

Methods for determining the relaxation spectrum can be divided into graphical, approximate analytical, and more accurate numerical methods. A comparative analysis showed that the numerical method of regularization is the most accurate, but in practice it is not applicable in the limited frequency range [2].

A modification of the numerical regularization method in problems of estimating the relaxation spectra of polymers is proposed. It consists in solving Fredholm integral equations of the first kind (1), and differs in applying extrapolation of experimental data based on a priori information about the type of polymer and its relaxation spectrum, which allows to calculate the spectrum from acoustic measurements.

$$G''(\omega)=\int_0^\infty H(\tau)\cdot\left(\frac{\omega\tau}{1+\omega^2\tau^2}\right)\frac{1}{\tau}d\tau=\sum_{i=1}^{n}g(\tau_i)\cdot\left(\frac{\omega\tau_i}{1+\omega^2\tau_i^{\,2}}\right),\quad H(\tau)=\sum_{i=1}^{n}\frac{g(\tau_i)}{\Delta\tau} \qquad (1)$$

where ω is the frequency, τ is the relaxation time, $G''(\omega)$ is the loss modulus, $g(\tau_i)$ is the discrete spectrum of relaxation times, n is the number of modes, $H(\tau)$ is the continuous spectrum.

To test the proposed method, a computational experiment was performed using the lognormal distribution function as an approximation of the relaxation spectrum. The results of the experiments showed that using the method of ultrasonic spectrometry and extending the interval with an extrapolation algorithm based on a priori information about the type of polymer, it is possible to restore the spectrum of relaxation times with an acceptable error. In this case, the error of the method largely depends on the choice of the extrapolating model.

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Preparation and Electrophysical Properties of a Mixed Ferroelectric Composite from Nanoparticles of Cellulose and Triglycine Sulfate

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In recent years, the tendency of using natural abundant materials for the synthesis of advanced materials in general or electronics materials in particular has been considered as a promising approach, for that nanocellulose $(C_6H_{12}O_6)_n$ is expected to be intensively used in the near future due to low-cost, high accessibility and environmental friendliness. In previous studies, the composites prepared from triglycine sulfate (TGS) imbedded into a matrix of nanoporous cellulose were synthesized and their electrophysical properties were studied quite thoroughly. In these composites, the ferroelectric phase region of TGS was expanded due to the strong interaction of hydrogen-containing TGS and cellulose through hydrogen bonds system. Besides, several interesting anomalies of dielectric relaxation were also detected. However, a huge drawback of porous nanocomposites is related to difficulties in controlling the content of ferroelectric inclusions, and therefore the effects of TGS content on properties of these materials were not reported. Luckily, this issue can be solved in the case of mixed nanocomposites, the components of which are precisely determined at the first stage of preparation process.

In this study, a novel ferroelectric composite consisting of triglycine sulfate (TGS) and cellulose nanoparticles (NCCP) prepared from waste cotton was synthesized and characterized by various techniques as X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and Zetasizer analyzer. The study on electrophysical properties of the composite samples at different weight composition ratios were performed from 25 to 120 °C under a weak electric field with an amplitude of 1 V/cm at low and infra-low frequencies (10^{-3} – 10^{3} Hz). The obtained results indicated that an increase in cellulose concentration in the composite led to increasing the phase transition temperature in TGS component from 3 to 63 ºC higher than those for single crystal TGS (+49 ºC). This anomaly was related to the interaction between TGS and cellulose nanoparticles through hydrogen bonds. Besides, at relatively high mass content of TGS (> 70%), an additional peak of dielectric constant was observed at higher temperature as compared to the lower-temperature one for the common ferroelectric phase transition, presumably, due to thermoactivation and redistribution of so-called B-centers in TGS. A significant dielectric dispersion detected at low and infra-low frequencies is explained by Maxwell-Wagner-Sillars interfacial mechanism.

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