XXII POLISH-CZECH SEMINAR

Structural and Ferroelectric Phase Transitions

BOOK of ABSTRACTS

Hucisko, Poland
May 16-20, 2016

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Structural and Ferroelectric Phase Transitions

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Organizers

Institute of Molecular Physics, Polish Academy of Sciences,
Mariana Smoluchowskiego 17, 60-179 Poznań, Poland
and
Institute of Physics, Academy of Sciences of the Czech Republic,
Na Slovance 2, 182 21 Prague 8, Czech Republic

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History of the Seminar

The idea of scientific meetings of physicists involved in studies of ferroelectrics in Poland and Czechoslovakia was born in the discussion between Bożena Hilczer and Jan Fousek, the heads of the ferroelectrics groups in both countries at that time. The regular meetings followed inevitably from the success of the first such event in Błażejewko, Poland in 1979. As always, the Seminar was organized by collaborating scientists from the Ferroelectrics Department of the Institute of Molecular Physics, Polish Academy of Sciences and Dielectric Department of the Institute of Physics, Czech Academy of Sciences.

We organize Seminars on Structural and Ferroelectric Phase Transitions, by turn, in Poland and in Czechoslovakia (now Czech Republic) to intensify the cooperation between the scientist of neighboring countries. We used to invite also our colleagues from other countries who we were collaborating with. The Seminars are the forum of presentation of recent results, unconstrained discussions and initiating of common studies. Lectures on general physics are also a custom of these meetings. The Seminars result not only in joint research and scientific integration but also in close friendship.

Previous Seminars

I	**Błażejewko, Poland**	**1979**
II	**Mělník, Czechoslovakia**	**1980**
III	**Kołobrzeg, Poland**	**1981**
IV	**Piesky, Czechoslovakia**	**1982**
V	**Kozubnik, Poland**	**1983**
VI	**Liberec, Czechoslovakia**	**1984**
VII	**Karpacz, Poland**	**1986**
VIII	**Senohraby, Czechoslovakia**	**1988**
IX	**Poznań-Kiekrz, Poland**	**1990**
X	**Paseky nad Jizerou, Czechoslovakia**	**1992**
XI	**Paseky nad Jizerou, Czechoslovakia**	**1994**
XII	**Jurata, Poland**	**1996**
XIII	**Liblice, Czech Republic**	**1998**
XIV	**Świnoujście, Poland**	**2000**
XV	**Nečtiny, Czech Republic**	**2002**
XVI	**Wierzba, Poland**	**2004**
XVII	**Znojmo, Czech Republic**	**2006**
XVIII	**Zakopane, Poland**	**2008**
XIX	**Telč, Czech Republic**	**2010**
XX	**Ustroń, Poland**	**2012**
XXI	**Sezimovo Ústi, Czech Republic**	**2014**
XXII	**Hucisko, Poland**	**2016**

Monday, May 16 Programme

15.00 - 18.00	**REGISTRATION**
18.00 - 18.15	**OPENING - B. Andrzejewski**
18.15 - 18.55	**J. Hlinka** - *Invited Lecture* **Multiferroics: how to switch them?**
19.00 -	**GET TOGETHER PARTY**

Tuesday, May 17 — Programme

Chairman	Time	Session
	8.00 - 9.00	**BREAKFAST**
Chairman - S. Kamba	9.00 - 9.40	**A. Bussmann-Holder** - *Invited Lecture* **$EuTiO_3$: a new route to achieve strong coupling multiferroicity**
	9.40 - 10.00	**V.V. Laguta** **Magnetic resonance study of the spin-spin interaction in $EuTiO_3$**
	10.00 - 10.20	**R.J. Radwański** **Magnetic phase transition in $EuTiO_3$ and $SrMnO_3$**
	10.20 - 10.40	**E. Langenberg Pérez** **Dielectric characterization of strained $(Sr_{1-x}Ba_x)MnO_3$ epitaxial thin films in the perovskite phase**
	10.40 - 11.00	**F.G. Figueiras** **Magnetoelectric effect enhanced by breaking the geometric magnetic frustration in $LuMn_{1+z}O_{3+\delta}$**
	11.00 - 11.30	**COFFEE**
Chairman - B. Dabrowski	11.30 - 12.10	**K. Szot** - *Invited Lecture* **Physics and chemistry at surfaces of model perovskite oxide**
	12.10 - 12.40	**K. Roleder** - *Key Lecture* *Simple or not simple* **antiferroelectricity?**
	12.40 - 13.00	**I. Bobowska** **Synthesis of zinc titanate on the textured substrate**
	13.00 - 13.30	**M. Paściak** - *Key Lecture* **Local structure and dynamics across the antiferroelectric phase transition in $PbZrO_3$**
	13.30 - 15.00	**LUNCH**

Tuesday, May 17 — Programme

	13.30 - 15.00	**LUNCH**
Chairman - Cz. Pawlaczyk	**15.00 - 15.40**	**T. Kopp** - *Invited Lecture* **Metallic states at $LaAlO_3/SrTiO_3$ interfaces**
	15.40 - 16.10	**J. Petzelt** - *Key Lecture* **Broadband dielectric spectroscopy of inhomogeneous and composite weak conductors**
	16.10 - 16.30	**A. Molak** **Electric current relaxations in $0.96BiMnO_3$-$0.04PbTiO_3$ ceramics annealed in N_2**
	16.30 - 17.00	**COFFEE**
Chairman - W. Schranz	**17.00 - 17.20**	**Z. Trybuła** **Coexistence of the relaxor-like and ferroelectric behavior in $K_{1-x}Li_xTaO_3$**
	17.20 - 17.40	**A. Naberezhnov** **Multiscale local ordering in uniaxial relaxor $Sr_{0.6}Ba_{0.4}Nb_2O_6$**
	17.40 - 18.00	**T. Sebastian** **Flexible ferroelectric hybrid fibres for soft body shape sensing**
	18.00 - 18.20	**O. Koleva** **Mixed valence influence on the structure of transition metal oxides**
	19.00 - 20.00	**DINNER**
	20.00 -	**POSTER SESSION**

Wednesday, May 18 — Programme

	Time	
	8.00 - 9.00	**BREAKFAST**
Chairman - J. Hlinka	9.00 - 9.40	**B. Dabrowski** - *Invited Lecture* Multiferroelectricity of corner-shared network of manganese and oxygen
	9.40 - 10.00	**V. Goian** Demonstration of spin-phonon coupling in infrared, THz spectra and microwave permittivity of $Sr_{1-x}Ba_xMn_{1-y}Ti_yO_3$ cermics and $Sr_{0.6}Ba_{0.4}MnO_3$ thin films
	10.00 - 10.20	**T.T. Carvalho** Role of La and Mn substitution on structure and electric properties of bismuth ferrite
	10.20 - 10.40	**P. Marton** Development of Landau potential for $BiFeO_3$
	10.40 - 11.00	**J. Kaczkowski** First-principles study of high-pressure phase of $BiGaO_3$
	11.00 - 11.30	**COFFEE**
Chairman - A. Kholkin	11.30 - 12.10	**S. Kamba** - *Invited Lecture* Soft modes in improper ferroelectrics and multiferroics
	12.10 - 12.40	**J. Pokorný** - *Key Lecture* Polarized Raman scattering on bismuth ferrite
	12.40 - 13.00	**K. Chybczyńska** High temperature dielectric response in size scaled $BiFeO_3$
	13.00 - 13.20	**A. Wypych-Puszkarz** Synthesis and dielectric investigations of $BaTi_4O_9$ obtained by soft chemistry route
	13.20 - 15.00	**LUNCH**

Wednesday, May 18 — Programme

	13.20 - 15.00	**LUNCH**
Chairman - J. Petzelt	15.00 - 15.40	**Ch. Simon** - *Invited Lecture* Neutron scattering in multiferroics: the example of $YMnO_3$
	15.40 - 16.10	**P. Fouquet** - *Key Lecture* Investigations of phase transitions on the nanometer scale by neutron spin echo spectroscopy
	16.10 - 16.30	**M. Kempa** Softening of elastic constants in relaxor PZN-8% PT by inelastic neutron scattering
	16.30 - 17.00	**COFFEE**
Chairman - K. Roleder	17.00 - 17.20	**P. Ławniczak** Universal features of conductivity spectra in some crystalline protonic conductors
	17.20 - 17.30	**M. Belyanchikov** Single-particle and collective states of water molecules in the matrix of beryl crystal lattice: experiment and theory
	17.30 - 17.40	**R. Vilarinho** Magnetoelectric mechanisms of slightly B-site doped $TbMnO_3$
	17.40 - 17.50	**I. Rafalovskyi** Macroscopic lamellar heterophase pattern in $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ single crystals
	17.50 - 18.00	**I. Niezgoda** Ester derivatives of 4-pentyl-4-hydroxyazobenzene - synthesis and characterization
	18.00 - 18.10	**S. Skiadopoulou** Magnetoelectric spin excitations in multiferroic Ni_3TeO_6
	18.10 - 18.20	**Ł. Lindner** Kinetics of phase transition in $(NH_4)_4H_2(SeO_4)_3$
	19.00 -	**GRILL PARTY**

Thursday, May 19 — Programme

	8.00 - 9.00	**BREAKFAST**
Chairman - Ch. Simon	**9.00 - 9.40**	**A. Kholkin** - *Invited Lecture* **Self-assembled peptides: structure, properties, applications**
Chairman - Ch. Simon	**9.40 - 10.00**	**M. Rok** **Structure and tunneling of methyl groups in molecular complexes containing 2-methylpyrazine, 2,3,5-trimethylpyrazine and organic acids**
Chairman - Ch. Simon	**10.00 - 10.20**	**A. Piecha-Bisiorek** **Multiferroicity in organic molecular-ionic salt**
Chairman - Ch. Simon	**10.20 - 10.40**	**M. Zdanowska-Frączek** **Electric conductivity and proton dynamics in superionic $(NH_4)_4H_2(SeO_4)_3$**
	10.40 - 11.10	**COFFEE**
Chairman - R. Świetlik	**11.10 - 12.50**	**K. Gallo** - *Invited Lecture* **Ferroelectric domain structuring for photonic applications**
Chairman - R. Świetlik	**12.50 - 12.20**	**T. Sluka** - *Key Lecture* **Charged domain walls in ferroelectrics**
Chairman - R. Świetlik	**12.20 - 12.40**	**P.S. Bednyakov** **Ultraviolet light induced formation of charged domain walls**
Chairman - R. Świetlik	**12.40 - 13.00**	**V. Stepkova** **Ising lines: natural topological defects within ferroelectric Bloch walls**
	13.00 - 14.30	**LUNCH**

Thursday, May 19 Programme

13.00 - 14.30	**LUNCH**
14.30 - 20.00	**EXCURSION**
20.00 - 21.00	**DINNER**

Friday, May 20 — Programme

	Time	
	8.00 - 9.00	**BREAKFAST**
Chairman - Z. Trybyła	9.00 - 9.30	**R. Świetlik** - *Key Lecture* Charge ordering and charge fluctuations in molecular conductors
	9.30 - 9.50	**A.V. Emelyanenko** Structure, elasticity and phase transitions in liquid crystals with deformations
	9.50 - 10.10	**Z. Galewski** 4'-(4-ethoxyazobenzene) alkanoates. Synthesis, mesomorphism and *trans-cis-trans* isomerisations
	10.10 - 10.30	**V. Bovtun** Broadband dielectric spectroscopy of $BaTiO_3$-$PbMg_{1/3}Nb_{2/3}O_3$ ceramics
	10.30 - 10.50	**I. Gregora** Hyper-Raman scattering in quest for A_u phonons in orthorhombic $PbZrO_3$
	10.50 - 11.10	**S. Krylova** Temperature Raman scattering study of BBN ceramics
	11.10 - 11.30	**COFFEE**
Chairwoman - M. Połomska	11.30 - 11.50	**I. Jankowska-Sumara** Phase transitions in $PbZr_{0.72}Sn_{0.28}O_3$ single crystals studied by Raman spectroscopy
	11.50 - 12.10	**F. Kadlec** Spin and lattice excitations in the room-temperature magnetoelectric $(Ba_{0.2}Sr_{0.8})_3Co_2Fe_{24}O_{41}$ with Z-type hexaferrite structure
	12.10 - 12.20	**CLOSING**
	12.20 - 13.30	**LUNCH**

POSTERS

P1 **M. Adamczyk-Habrajska**
Dielectric and semiconductor properties of $(Ba_{0.6}Pb_{0.4})TiO_3$ ceramics doped with glass in the range of phase transition

P2 **A. Almeida**
Structure and physical properties of $Ca_{1-x}Sr_xMn_7O_{12}$

P3 **A. Bubnov**
New smart liquid crystalline polymethacrylates highly photosensitive in a broad spectral range

P4 **A. Bubnov**
Self-assembling photosensitive materials as functional dopants for organic photovoltaic cells

P5 **R. Bujakiewicz-Korońska**
X-ray characterization of Co doped tetragonal $BaTiO_3$ ceramics

P6 **J. Dec**
Optical quasi-biaxiality of relaxor strontium-barium niobate single crystals

P7 **Z. Dočekalová**
Predicted infrared spectra of PZO phonons

P8 **J. Drahokoupil**
Phase transition in multiferroic Ni-Mn-Ga single crystal

P9 **E.M. Dutkiewicz**
Phase transition, thermal, Raman and dielectric characteristics of lead-free $(1-x)Na_{0.5}Bi_{0.5}TiO_3$-$xSrTiO_3$ (x=0, 0.08 and 0.1) ceramics

P10 **J. Fábry**
Suggestion of the extension of the defintion of a chemical reaction

P11 **S. Fedyk**
Antiferromagnets and ferrimagnets in high magnetic fields

P12 **B. Garbarz-Glos**
Dielectric properties of potassium-sodium niobate ceramics at low frequencies

P13 **M. Glogarová**
Frustrated smectic liquid crystalline phases in lactic acid derivatives

P14 **W. Głuchowski**
Mechanical properties and superconducting nanostructures of Cu-Ag and Cu-Nb thin wires

P15 **A. Hilczer**
Structure and magnetic properties of Nd and Al codoped $SrFe_{12}O_{19}$

P16 **S. Kamba**
Broad-band dielectric response of $0.5Ba(Ti_{0.8}Zr_{0.2})O_3$-$0.5(Ba_{0.7}Ca_{0.3})TiO_3$ ceramics: soft and central mode behavior

POSTERS

P17 **M. Karpierz**
Effects of $PbTiO_3$ doping on electric properties of $Na_{0.5}Bi_{0.5}TiO_3$ ceramics

P18 **A. Klíč**
Dielectric properties of stratified polydomain $BiFeO_3$

P19 **K. Konieczny**
Electrical and thermal properties of $Na_{1-x}Li_xNbO_3$ (x = 0.08, 0.1, and 0.2) ceramics near the morphotropic phase boundary

P20 **L. Kozielski**
Double hysteresis loop in $BaTiO_3$-based ferroelectric ceramics prepared by high energy milling

P21 **W. Kuczyński**
The influence of the dye concentration on the liquid crystals' order parameter $\langle P_2 \rangle$

P22 **A. Leonarska**
Structural, electric and Mössbauer studies of 5% Fe - doped $BiMnO_3$

P23 **U. Lewczuk**
Dielectric and ferroelectric properties of NBT-BT systems

P24 **E. Markiewicz**
Dielectric and magnetic properties of $BiFeO_3$-PVDF nanocomposites

P25 **A. Naberezhnov**
Ferroelectric nanocomposites on base of magnetic porous glasses

P26 **D.M. Nalecz**
The crystal field effects in hexagonal 4H-$SrMnO_3$

P27 **D. Nicheva**
Synthesis and structure studies of $Ni_xCo_{3-x}O_4$

P28 **A. Nikolaienko**
The creation of static atomic displacement waves in irradiated $TlInS_2$ crystals

P29 **V. Novotná**
Liquid crystalline derivatives with terphenyl molecular core and lactic acid unit as chiral moiety

P30 **K. Nowicka**
Physical properties of prepared liquid crystal mixtures forming the blue phases

P31 **D. Nuzhnyy**
Effective dielectric function of $BaTiO_3$-NiO nano-composites

P32 **P. Ondrejkovic**
Polarization fluctuations in SBN single crystals

P33 **Cz. Pawlaczyk**
Universality of conductivity spectra in superprotonic $(NH_4)_3H(SO_4)_2$ single crystal

POSTERS

P34 **A. Pawłowski**
Impedance spectroscopy study of $(NH_4)_3H(SeO_4)_2$: evidence of increase in lattice disorder in the low temperature phases

P35 **P. Perkowski**
Dielectric properties of new fluorinated compounds exhibiting ferro- and antiferroelectric phases

P36 **J. Piecha**
Structural and electrical features induced by leaching procedures on $LiNbO_3$ crystalline powder samples

P37 **M. Pilch**
Influence of thermal treatment on properties of $BiMnO_3$ ceramics

P38 **K. Pogorzelec-Glaser**
Spectral investigations of proton conducting material $(IMD)_2SeO_4 \cdot 2H_2O$

P39 **M. Połomska**
XRD, Raman and magnetic studies of $Bi_{1-x}La_xFeO_3$ solid solution obtained by mechanochemical synthesis

P40 **J.K. Prytys**
Flexible crystals of perovskite-like coordination polymers with tunable and switchable organic guest

P41 **S. Puchberger**
Avalanche critical exponents in nanoporous systems under compression

P42 **K. Pytel**
Basic characterization and standard dielectric measurements on PLZT x/65/35 ceramics based on correlation coefficients

P43 **S.A. Różański**
Dynamics of collective modes in ferroelectric liquid crystal gels

P44 **I. Rychetsky**
Relationship between dielectric and elastic properties of the porous ceramics

P45 **M. Savinov**
Broadband dielectric spectroscopy of the non-relaxor $PbFe_{1/2}Ta_{1/2}O_3$ ceramics

P46 **W. Schranz**
On the behaviour of liquids and polymers in nano-confinement

P47 **D.V. Shmeliova**
Orientational fluctuations and phase transitions in 8CB confined by cylindrical pores of PET film

P48 **D. Sitko**
Effect of uniaxial stress on the dielectric properties of $BaTiO_3$+0.1%Eu ceramics

POSTERS

P49 **Z. Slavkova**
High temperature study of $LiNaSO_4$

P50 **J. Suchanicz**
Dielectric, thermal and Raman properties of lead-free $(Na_{0.5}Bi_{0.5})_{1-x}Sr_xTiO_3$ (x=0, 0.04 and 0.06) ceramics

P51 **I. Szafraniak-Wiza**
Physical properties of nanosized $Ba_{1-x}Ca_xTiO_3$ solid-solid solution obtained by mechanochemical synthesis

P52 **I. Szafraniak-Wiza**
Preparation and properties of Bi_3TiNbO_3 obtained by conventional solid state reaction and mechanochemical synthesis

P53 **A. Szeremeta**
Electrical properties of epoxy-glue / $BiMnO_3$ composite

P54 **M. Trybus**
Phase transition in triglycine sulphate under dynamic stimulation

P55 **M. Wojciechowska**
Isomorphous structural phase transition and properties of new diisobutylamine-based molecular-ionic salt

P56 **M.B. Zapart**
Phase transformations of $KSc(WO_4)_2$: domain structure and X-ray studies

P57 **W. Zapart**
Optical studies of the ferroelastic phase transitions in $KFe(MoO_4)_2$

P58 **V. Železný**
Infrared spectroscopy of strained $BaTiO_3/SrTiO_3$ superlattices on $DyScO_3$ substrates

P59 **J. Agostinho Moreira**
Experimental evidence of a twofold order-disorder structural phase transition sequence in perovskite-like $[(CH_3)_2NH_2][Mn(HCOO)_3]$

LECTURES

INVITED LECTURE

MULTIFERROICS: HOW TO SWITCH THEM?

J. Hlinka
Institute of Physics, The Czech Academy of Sciences, Na Slovance 2, 182 21 Prague 8, Czech Republic
hlinka@fzu.cz

Multiferroic materials are currently often considered among the top research topics in the field of the structural and magnetic phase transitions. In the past, the term multiferroic was often used to indicate simultaneous presence of two or more primary spontaneous quantities, conjugated to the electric, magnetic or stress field. Hans Schmidt, one of the pioneer of the field of the magnetoelectric crystal properties, proposed to extend the list of such primary ferroics by including also ferrotoroidics, materials with spontaneous magnetic toroidal moment [1]. This immediately suggests that the so-called ferroxial materials, with spontaneous electric toroidal moment [2] are equally eligible as primary ferroics, too.
Actually, definitions adopted in the International tables of crystallography generalized the original Aizu definition in a way that the ferroic phase simply means the low-symmetry phase, resulting from any kind of phase transition, associated with the point group symmetry-breaking.
Whatever definition we adhere to, the multiferroics of all kinds are around us. The more exotic order parameters are involved, the more intriguing can be the issue of the domain switching. We wish to discuss the usual attitudes to the symmetry breaking in material science and to provide few simple ideas that can be useful to deal with properties of structurally complex ferroelectric, antiferroelectric or multiferroic single crystal materials. We shall also argue that the signature of the proper ferroelectric Bloch wall is an emergent chirality, i.e. the chirality that appear as a consequence of a continuous symmetry-breaking transition within the wall [3,4].

References

[1] Schmid H: On Ferrotoroidics and Electrotoridic, Magnetotoroidic and Piezotoroidic Effects. Ferroelectrics 2001;252:41

[2] Hlinka J: Phase-field modelling of 1800 "Bloch walls" in rhombohedral $BaTiO_3$. Phys. Rev. Lett. 2014;113:165502

[3] Stepkova V, Marton P and Hlinka J: Stress-induced phase transition in ferroelectric domain walls of $BaTiO_3$. J. Phys.: Condens. Matter 2012;24:212201

[4] Hlinka J, Stepkova V, Marton P and Ondrejkovic P: Ferroelectric domain walls and their intersections in phase-field simulations. In: Seidel J, eds. Topological structures in ferroic materials. Switzerland: Springer International Publishing; 2016;161

INVITED LECTURE

$EuTiO_3$: A NEW ROUTE TO ACHIEVE STRONG COUPLING MULTIFERROICITY

A. Bussmann-Holder
Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany
a.bussmann-holder@fkf.mpg.de

Multiferroic materials with combined polar, magnetic, and elastic orderings are at the forefront of scientific research in view of their complex interactive couplings: magnetic order can be tuned by strain and an electric field, polar order can be triggered by a magnetic field and strain, and elastic properties are controlled by a magnetic and/or an electric field. Such materials are desirable for multiple applications. Even though the phenomenon of multiferroicity has been predicted long ago [1], its realization remains rare for rather simple reasons: typically polar order is achieved when a transition metal d0 configuration is combined with highly polarizable anions, whereas magnetic order relies on a finite dn configuration. Obviously these two requirements yield a certain incompatibility for the coexistence of the two phenomena which have been tried to overcome by combining magnetic layers with polar ones, by growing composites, and via strain engineering [2,3]. Even though a rather large number of materials have been shown to exhibit the desired properties, the coupling between magnetic and polar order is either very weak, or the spontaneous polarization/magnetization appears at low temperature only and remains too small to be of technological interest. Here we propose a new strategy to achieve strong magnetic-polar coupling by deriving the soft mode frequency of $EuTiO_3$ as a function of its lattice parameter which exhibits unusual, yet very small temperature dependencies at high and low temperatures [4,5]. Specifically we develop a route of how to induce ferroelectric order in bulk $EuTiO_3$ (ETO) by combining experimental results with theoretical concepts. We show that marginal changes in the lattice parameter of the order of 0.01% have a more than 1000% effect on the transverse optic soft mode of ETO and thus easily induce a ferroelectric instability [6].

References

[1] Smolenskii GA, Isupov VA, & Agronovskaya AI, Sov. Phys Solid State, **1**, 149 (1959)

[2] Erenstein W, Mathur ND, & Scott JF, Nature **422**, 759-765 (2006)

[3] Ramesh R, & Spaldin NA, Nature Materials **6**, 21 (2007)

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[5] Reuvekamp PG, Kremer RK, Köhler J, & Bussmann-Holder A, Phys. Rev. B **90**, 104105 (2014)

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MAGNETIC RESONANCE STUDY OF THE SPIN-SPIN INTERACTION IN $EuTiO_3$

V.V. Laguta[1], S. Kamba[1], B. Andrzejewski[2], M. Kachlík[3], K. Maca[3], J.H. Lee[4] and D.G. Schlom[4]

[1]*Institute of Physics ASCR, Na Slovance 2, 18221 Prague 8, Czech Republic*

[2]*Institute of Molecular Physics PAS, Smoluchowskiego 17, 60-179 Poznań, Poland*

[3]*Brno University of Technology, Technická 2, 61669 Brno, Czech Republic*

[4]*Cornell University, Ithaca, New York, 14853-1501, USA*

laguta@fzu.cz

$EuTiO_3$ is a frequently investigated material in the last decade due to the discovery of relatively strong magnetoelectric (ME) effect below the antiferromagnetic (AFM) phase transition temperature $T_N \approx 5.4$ K, where the dielectric permittivity decreases almost 5% on cooling below T_N and increases 7% with rising magnetic field [1]. It is an incipient ferroelectric, like $SrTiO_3$ because quantum fluctuations suppress possible ferroelectric phase transition at low temperature. However, recently, it was found that both ferroelectric and ferromagnetic order can be induced by biaxial strain in thin $EuTiO_3$ films [2] that opens a new route for construction of novel multiferroic nanostructures with a strong ME coupling. There are numerous studies on this material in the form of ceramics, crystals and thin films grown on different substrates (see e.g. [1-4]). In particular, ceramic samples of $EuTiO_3$ were also studied by electron paramagnetic resonance [3], but only in the paramagnetic phase down to about 50 K. To the best of our knowledge, this material was never studied using conventional magnetic resonance technique in the magnetically ordered phase, especially in the form of thin film.

In this work we present a detailed study of the magnetic resonance spectra in $EuTiO_3$ bulk samples and 100 nm thickness epitaxial film grown on $DyScO_3$ substrate in wide temperature region from 350 down to 3 K at microwave frequencies 9.2 - 9.8 and 34 GHz. We have found that in the paramagnetic phase magnetic resonance spectra are determined by magnetic dipole and exchange interactions between Eu^{2+} spins. In film, the large contribution from demagnetization field is presented. From analysis of linewidth and its temperature dependence, the parameters of spin-spin interactions were determined: the exchange frequency is 15 - 15.5 GHz and the estimated critical exponent of the spin correlation length is ≈ 0.5. The spectra show distinct minimum in the linewidth at the Neel temperature $T_N \approx 5.4$ K while the resonance field practically does not change even with cooling far below this temperature indicating a small magnetic anisotropy ~320 G. The magnetic resonance spectrum in film is split into several components due to excitation of the magnetostatic modes corresponding to non-uniform precession of magnetization. The film shows aged effect that results in increase of crystal structure imperfections and decrease of the sublattice magnetization to 450 emu/cm^3 or 5.5 μB/unit cell.

References

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MAGNETIC PHASE TRANSITION IN $EuTiO_3$ AND $SrMnO_3$

R.J. Radwanski[1,2], Z. Ropka[2] and D.M. Nalecz[1]
[1]*Institute of Physics, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*
[2]*Center of Solid State Physics, S^{nt} Filip 5, PL-31150 Krakow, Poland*
sfradwan@cyf-kr.edu.pl

Perovskites are known to form the biggest group of ferroelectrics. Here $BaTiO_3$, $CaTiO_3$, $SrTiO_3$, $PbTiO_3$, $LiNbO_3$ can be mentioned. All of these compounds can be regarded as having only core closed electronic shells.
In this contribution we would like to analyze magnetic phase transitions in $EuTiO_3$ and in $SrMnO_3$. In these perovskite oxides there are magnetically active ions, Eu and Mn, which have an incomplete 3*d* shell. They exhibit the magnetic order at 5.5 K [1] and 233 - 286 K (depending on the polymorh type) [2,3], respectively.
The detailed specific-heat measurements presented in Ref. 1 allows for unambiguous determination of the entropy related with the magnetic phase transition owing to the low temperature of the transition - then the lattice contribution is small. The Eu^{2+} and Mn^{4+} ions are somehow similar in the respect that in the magnetic phase transition practically only spin degree of freedom are released. We have calculated temperature dependence of the specific heat including λ-type peak [4] and of the low-energy atomic-like electronic structure at the sub-meV energy scale. In the magnetic state there exists the discrete atomic-like electronic structure at the 0.05 meV scale. Our studies establish that the realized valency of the Eu^{2+} and Mn^{4+} in these oxides is exactly the same as the formal valency. We compare the derived molecular field acting on the Eu^{2+} and Mn^{4+} ion with exchange parameters J_{nn} and J_{nnn} derived in Ref. 6.

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DIELECTRIC CHARACTERIZATION OF STRAINED $(Sr_{1-x}Ba_x)MnO_3$ EPITAXIAL THIN FILMS IN THE PEROVSKITE PHASE

E. Langenberg[1,2], L. Maurel[2,3], R. Guzmán[3,4], J. Blasco[1,2], C. Magén[3,4,5], P.A. Algarabel[1,2] and J.A. Pardo[3,4,6]

[1]*Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza-CSIC, 50009 Zaragoza, Spain*

[2]*Departamento de Física de la Materia Condensada, Universidad de Zaragoza, 50009 Zaragoza, Spain*

[3]*Instituto de Nanociencia de Aragón, Universidad de Zaragoza, 50018 Zaragoza, Spain*

[4]*Laboratorio de Microscopías Avanzadas, Instituto de Nanociencia de Aragón, Universidad de Zaragoza, 50018 Zaragoza, Spain*

[5]*Fundación ARAID, 50004 Zaragoza, Spain*

[6]*Departamento de Ciencia y Tecnología de Materiales y Fluidos, Universidad de Zaragoza, 50018 Zaragoza, Spain*

eric.langenberg.perez@gmail.com

The possibility of controlling the magnetization (polarization) by an electric (magnetic) field in materials displaying ferroelectric and magnetic order in the same phase, so-called multiferroic materials, has triggered great amount of research in the last few years. However, very few of them have been proved to show strong magnetoelectric coupling, mainly due to the different mechanisms of ferroelectricity and magnetism in these compounds. Exception can be found, though, in perovskite $AMnO_3$ system (A = Ca, Sr, Ba), in which Mn^{4+} is expected to be able to drive both the magnetic order and the required non-centrosymmetric distortion for ferroelectric order. Yet ferroelectricity is allowed in this system, solely, when the unit cell volume is large enough to promote Mn off-centring [1], which may be achieved by using increasingly larger A cation, as partially replacing Sr with Ba [2], or artificially expanding the lattice parameters by epitaxial strain engineering [3]. However, increasing the size of the A-cation destabilizes the perovskite structure, becoming different non-ferroelectric hexagonal polymorphs the ground state phase [4].

Epitaxial $(Sr_{1-x}Ba_x)MnO_3$ thin films, Ba content ranging $0.2 \leq x \leq 0.5$, were grown by pulsed laser deposition onto a wide variety of different (001)-oriented perovskite substrates spanning a misfit strain from 0% to 4%. X-ray diffraction measurements show that the perovskite phase is stabilized over the non-ferroelectric hexagonal phase and that the films grow fully coherent on the perovskite substrates [5]. Electrical measurements based on impedance spectroscopy have been performed to assess the dielectric properties of $(Sr_{1-x}Ba_x)MnO_3$ films as a function of Ba-content and epitaxial strain, covering a wide range in this 2D phase diagram. Impedance spectroscopy methods allow disentangling extrinsic contributions to the measured capacitance and to extract the temperature dependence of the intrinsic dielectric and resistive properties of the strained films [6]. Results show that a pronounced dielectric anomaly appears above room temperature when either strain or Ba-content is increased, which we ascribed to the enhancement of the polar character of the films.

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MAGNETOELECTRIC EFFECT ENHANCED BY BREAKING THE GEOMETRIC MAGNETIC FRUSTRATION IN $LuMn_{1+z}O_{3+\beta}$

F.G. Figueiras[1,2], D.V. Karpinsky[1], P. Tavares[3], S.Y. Vilar[2], A.F.M. Santos[4], M. Tovar[5], J. Agostinho Moreira[2] and V.S. Amaral[1]

[1]*Physics Department & CICECO-AIM, Aveiro University, 3810-193 Aveiro, Portugal*

[2]*IFIMUP-IN, Science Faculty; Porto University, 4169-007 Porto, Portugal*

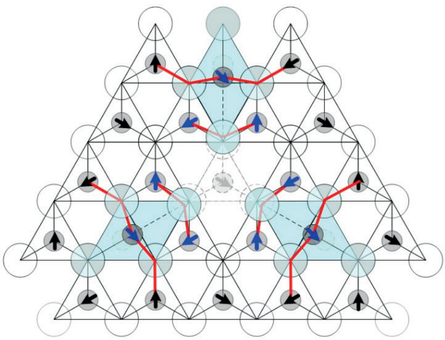
[3]*Chemistry Center, Trás-os-Montes & Alto-Douro University, 5001-801 Vila Real, Portugal*

[4]*SNS, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, USA*

[5]*Helmholtz Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany*

ffigueiras@ua.pt

A comprehensive insight of the structural and properties effects due to controlled off-stoichiometry in the $LuMn_{1+z}O_{3+\delta}$ (**z** = -0.02; **δ** ~ 0) hexagonal manganite is supported by Neutron Powder Diffraction measurements confirming single phase hexagonal structure and exposing, below $T_{Néel}$ ~90 K, a pertinent ferromagnetic component which breaks the archetypal geometrical frustrated antiferromagnetic state ascribed for the utter $LuMnO_3$ compound [1]. The evaluated triangular disposition of spins prompts an electric polarization contribution [2] and a clear enhancement the magnetoelectric effect [3]. In addition, Raman spectroscopy, dielectric, pyroelectric and magnetic measurements as function of temperature enabled to recognize intrinsic interaction between structural, transport and magnetic contributions, well



above Néel transition.

Fig. 1. Diagram of the basal plane of the $LuMnO_3$ and the local disturbance prompt by a Mn vacancy in the antiferromagnetic geometric frustration.

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INVITED LECTURE

PHYSICS AND CHEMISTRY AT SURFACES OF MODEL PEROVSKITE OXIDES

K. Szot
Institute of Physics, University of Silesia, 40-007 Katowice, Poland
k.szot@fz-juelich.de

The surface of ABO_3 crystals with perovskite structure constitutes, just like in other solids, a native boundary between the crystal and its surroundings. When the surface of the crystals is created as an effect of natural growth, cutting, polishing, or etching the translational perfection of the bulk as well its electronic properties, the lattice dynamics, the transport properties (e.g., electrical, thermal, diffusion) are modified at the surface. In most cases, the surfaces of ternary oxides are prepared ex situ. Therefore, this preparation step leads to a dissonance between the interpretation of the properties of a "clean" surface (generated via in situ treatment) versus the understanding of properties of a "dirty" (ex situ prepared) real surface layer. In fact, additional layer(s) of physisorbates and chemisorbates do not only modify the physical properties of the "dirty" (contaminated) layer but the interaction of the surface with the environment can even induce a change of the chemical composition of the surface layer [1]. Without doubt, the most massive transformation on the surface layer of ABO_3 oxides with perovskite structure can be introduced by so-called redox reactions [1,2]. Driving forces for such reactions are: low oxygen partial pressure (vacuum, reduction gases) and elevated temperature. In particular the high concentration of the extended defects in the surface layer (surface region), which can act as an easy transport paths for ions, can "accelerate" the restructuring of the outer part of the crystal [1,3]. Irradiations of the surface under vacuum conditions with photons, electrons, or ions can cause a similar change of the oxidation state of the transition metal ions as the redox reactions. It is surprising that a seemingly harmless deposition of metallic electrodes can induce, via transfer of a huge momentum of metal atoms (cluster) on ions in the surface layer (especially oxygen ions), an effect similar to reduction and segregation. In my lecture I will show that the details of the physical and chemical nature of the surface layer, which has been introduced as a concept by Känzing [4] in the 1950s (so-called surface skin of $BaTiO_3$), can be now better understood using the modern surface sensitive techniques on the atomic scale.

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Permanent address: Peter Grünberg Institute, Forschungszentrum Jülich, D-52-428 Jülich, Germany.

KEY LECTURE

SIMPLE OR NOT SO SIMPLE **ANTIFERROELECTRICITY?**

K. Roleder
University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland
Krystian.Roleder@us.edu.pl

In spite of over 60 years of investigations concerning antiferroelectricity in oxidic perovskites ABO_3, it cannot be claimed that we fully understand the phase transition mechanisms leading to this state. Lead zirconate $PbZrO_3$ belongs to the so called classical (*simpl*e) aniferroelectrics, and has been intensively studied in the last few years [1-4]. Experiments have been made on the purest crystal we had to now. These experiments have proved that the Curie-Weiss law is not fulfilled in wide temperature range. It was also established that above T_C there is the temperature T_{BH} below which fluctuations of local polarity starts appearing. Moreover, inside the (T_C - T_{BH}) range there is a temperature point below which permanent polar regions exist and grow up while approaching to transition point.

All the statements above are in favour of not so simple mechanism leading to antiferroelectric order. It would not have been considered, if earlier investigations on so-called pre-transitional phenomena in $BaTiO_3$ [5] and $SrTiO_3$ [6,7] had not been detected. While the static and birefringent micro-regions were visible above T_C in $BaTiO_3$, which is entirely ferroelectric below T_C, considerably different behaviour was observed in the case of $SrTiO_3$, in which precursor effects are related to long wavelength and zone boundary acoustic modes instabilities, and exist even 60 K above transition point.

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SYNTHESIS OF ZINC TITANATE ON THE TEXTURED SUBSTRATE

I. Bobowska[1], A. Wypych-Puszkarz[1], A. Opasińska[1], W. Maniukiewicz[2], P. Wojciechowski[1] and J. Ulański[1]

[1]*Department of Molecular Physics, Lodz University of Technology, Lodz, Poland*

[2]*Institute of General and Ecological Chemistry, Lodz University of Technology, Lodz, Poland*

izabela.bobowska@p.lodz.pl

Zinc titanates attract the attention because of their importance in practical applications. $ZnTiO_3$ is commonly known as low-temperature sintering dielectrics [1]. In coating form this compound is a good candidate as solid lubricant at high temperatures up to 550 °C [2]. Zn_2TiO_4 is used as high temperature regenerable catalyst and sorbent of sulphur from coal gasification products as well as it may also be applied as photocatalyst in water splitting or organic compounds degradation. Annealing of the ZnO-TiO_2 system leads to one or more of the known phases: $Zn_2Ti_3O_8$ that is metastable low-temperature form of $ZnTiO_3$ with a cubic defect spinel structure; zinc methatitanate $ZnTiO_3$ with rhombohedral ilmenite structure; zinc orthotitanate Zn_2TiO_4 with a cubic spinel crystal structure [3]. The crystal structure of zinc titanate and presence of impurities like ZnO and TiO_2 is determined by Zn:Ti ratio and sintering conditions. Typically, zinc titanate can be prepared by ball milling of ZnO and TiO_2 powder and subsequent sintering. Obtained product can be in a powder form or self-supporting plate. The ball-milling process is intended to mix reagents and mechanically activate the surface of adjacent grains. The milling is not necessary when chemical methods are applied, such as sol-gel or Pechini process, that ensure molecular mixing of reactants, but thermal treatment is still required in order to crystallize zinc titanate phase. Mentioned methods do not allow to control texture of growing phases. It was reported, that the texture of $ZnTiO_3$ layers, obtained via atomic layer deposition, can influence their mechanical properties [2]. Here we propose a utilization of textured ZnO substrate as a precursor of zinc titanate layers. The main aim of the present study was to synthesize layers of zinc titanate by thermal treatment of nanocomposite of ZnO nanorods coated with layered tetramethylammonium titanate (LTMAT). The ZnO nanorod arrays were obtained by chemical bath deposition method [4]. The LTMAT was prepared according to Ohya et al. [5] and used as water soluble TiO_2 precursor. The layers of ZnO nanorods/LTMAT were subjected to heat treatment. Phase composition after sintering was analyzed using X-ray diffraction method whereas microstructure analysis was performed via scanning electron microscope.

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KEY LECTURE

LOCAL STRUCTURE AND DYNAMICS ACROSS THE ANTIFERROELECTRIC PHASE TRANSITION IN $PbZrO_3$

M. Paściak[1], T.R. Welberry[2], S. Leoni[3] and J. Hlinka[1]

[1]*Institute of Physics, Czech Acad. Sci., Na Slovance 2, 18221 Prague 8, Czech Republic*

[2]*Research School of Chemistry, Australian National University, Canberra ACT 0200, Australia*

[3]*Cardiff University, School of Chemistry, Cardiff, UK*

pasciak@fzu.cz

The principles of antiferroelectric (AFE) phase transitions have been recently explored in studies concerning critical behaviour of $PbZrO_3$ (PZO). Two different explanations for simultaneous freezing of three lattice modes leading to AFE phase have been offered, putting accents either on the primary role of the ferroelectric soft mode [1] or on the trilinear coupling of all distortions [2]. Additionally, some precursor phenomena and an intermediate phase have been identified, indicating rich local structural phenomena accompanying the transition. This has been further confirmed in our recent works [4,5] where we have concentrated on the structured diffuse scattering coming from local distortions in cubic PZO. An ab-initio based shell model has been developed to help us analyzing the data and allow an insight into the dynamical characteristic of the observed features. We identify effects related to different modes and track their changes across the phase transition. The results are discussed in the broader context of other lead containing perovskites, especially relaxor ferroelectrics.

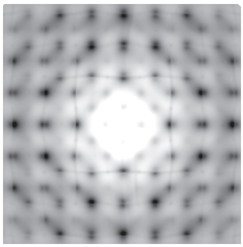

Fig. 1. Diffuse scattering on the *hk*0.5 reciprocal plane in the cubic phase of PZO comprising features related to correlated shifts of Pb atoms (intense blobs) as well as octahedra tilting (weak but sharp lines).

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INVITED LECTURE

METALLIC STATES AT $LaAlO_3/SrTiO_3$ INTERFACES

T. Kopp
Center for Electronic Correlations and Magnetism, Institute of Physics University of Augsburg, Augsburg, Germany
thilo.kopp@physik.uni-augsburg.de

Breaking the translation or inversion symmetry at surfaces and interfaces may lead to the formation of charge, spin and orbital electronic states which do not exist in the bulk. The emergence of these states is particularly relevant for oxides where the balance of competing interactions and the resulting stable electronic phase crucially depend on the local oxidation state near the interface. A prominent example is the interface of $LaAlO_3/SrTiO_3$ (LAO/STO). The formation of a metallic state at the interface of the band insulators LAO and STO has become a prototype for the reconstruction of electronic states which exhibit a variety of phenomena such as negative compressibility, superconductivity, and magnetism. The metallic states have been investigated by tuning the charge carrier concentration with transverse electric fields.

KEY LECTURE

BROADBAND DIELECTRIC SPECTROSCOPY OF INHOMOGENEOUS AND COMPOSITE WEAK CONDUCTORS

J. Petzelt and D. Nuzhnyy
Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Prague 8, Czech Republic
petzelt@fzu.cz

In this review we will discuss broadband dielectric spectroscopy from mHz up to near infrared range (10^{-3} - 10^{15} Hz, i.e. up to 18 orders of magnitude in frequency) mainly in materials with inhomogeneous but weak conductivity, including conductor-dielectric nanocomposites. Our discussion is based on the effective medium approach (EMA) [1] and mainly experiments based on this approach are reviewed. The advantages of EMA models compared to frequently used approaches based on electrical equivalent circuits are discussed. The EMA enables to separate additively the response of percolated parts, which are not influenced by the depolarizing field, and nonpercolated parts, which are variously influenced by the depolarizing field depending on the topology and shapes of individual homogeneous parts [2,3]. We shall separately discuss core-shell composites, in which the cores are not percolated at all, and normal composites with a possible percolation of the conductor component resulting in smeared or sharp percolation threshold of the DC conductivity and diverging static permittivity in the latter case. In the case of conductor core - dielectric shell the percolation is approached for the shell thickness approaching zero, connected with the diverging static permittivity (barrier-layer capacitors, giant permittivity effects). The sharp percolation threshold can be modelled by the well-known Bruggeman EMA model (with the percolation threshold of 1/3 for spheres) or by general effective medium approach with arbitrary percolation threshold and arbitrary critical exponents of the DC conductivity and static permittivity [4]. The best model for smeared percolation threshold with complex topology and shapes of components appears to be the general Lichtenecker model with positive exponent α allowing for partial percolation of both components for any composition [2,3,5]. Finally, numerous papers reporting negative low-frequency permittivity in weakly conducting materials are discussed and it is concluded to be spurious effects due to artifacts of improper measurements or inappropriate measurements technique [6].

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ELECTRIC CURRENT RELAXATIONS IN $0.96BiMnO_3$-$0.04PbTiO_3$ CERAMICS ANNEALED IN N_2

A. Molak
Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland
andrzej.molak@us.edu.pl

The $0.96BiMnO_3$-$0.04PbTiO_3$ ceramics were sintered at 1170 K in ambient air from non-polar bismuth manganite [1] and ferroelectric lead titanate [2] components. The ceramics consists of two centrosymmetric phases: orthorhombic *Pbmn* and a sillenite cubic *I23* [1]. SEM analysis exhibited irregular polyhedron-type shapes of the ceramics grain. Non-homogeneous chemical composition was determined [3]. The samples were annealed in nitrogen N_2 flow at 1120 K. The electric impedance was measured for f = 100 Hz - 1 MHz in the 100 - 650 K range. It was analysed with use of electric modulus M"(T,f) formalism [4,5]. Two relaxation processes occurred in the as-sintered $BiMnO_3$-$PbTiO_3$ ceramics [1,6]. One process, which shown characteristic time value $\tau_{0,1} \approx 10^{-11}$ s and activation energy $E_{a,1} = 0.15$ eV, occurred in 110 - 220 K range. Next process occurred in 10 - 300 K range and it shown $\tau_{0,2} \approx 10^{-13}$ s and $E_{a,2} = 0.39$ eV. The third process appeared in 290 - 400 K range. It was enhanced after annealing in N_2 and it exhibited $\tau_{0,3} \approx 10^{-12}$ s and $E_{a,3} = 0.5$ - 0.6 eV. The dc resistivity $\rho_{dc}(T)$ shows semiconductor features in 200 - 750 K range. The variable range hopping of small polaron mechanism of conductivity occurred below room temperature. The annealing induced a slight increase in ρ_{dc} value and in value $E_{a,dc} = 0.4$ - 0.6 eV. The structural disorder varied due to the annealing [3]. Hence, the electric features were affected by the annealing in nitrogen.

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COEXISTENCE OF THE RELAXOR-LIKE AND FERROELECTRIC BEHAVIOR IN $K_{1-x}Li_xTaO_3$

Z. Trybuła[1], J. Dec[2], S. Miga[2], Sz. Łoś[1] and M. Trybuła[1]
[1]*Institute of Molecular Physics, Polish Academy of Science, PL-60-179 Poznań, Poland*
[2]*Institute of Materials Science, University of Silesia, PL-40-007 Katowice, Poland*
trybula@ifmpan.poznan.pl

The potassium tantalate crystal $KTaO_3$ belongs to the perovskite family of the general formula ABO_3 (A= Ba, K, Sr, Ca; B= Ti, Ta). This class of materials are still important because of a broad range of physical properties: relaxor, ferroic, multiferroic [1] or even superconducting behavior [2]. Nominally pure, so call quantum paraelectric or incipient ferroelectric potassium tantalate $KTaO_3$, has polar soft TO_1 transverse optic mode, which is stabilized by the zero- point quantum fluctuations of atoms and thus prevents the softening of TO_1, and do not exhibit ferroelectric phase transition down to a very low temperatures, experimentally to 0.003 K, and remain in the paraelectric cubic phase [3]. $KTaO_3$ has a highly polarizable lattice and is sensitive to impurities and defects [1]. Recently, evidence of polar nanoregions (PNRs) in nominally pure $KTaO_3$ crystals [4], and a strain-induced ferroelectric order in epitaxial thin film of $KTaO_3$ [5] have been reported. A particular attention is paid to the lithium-doped potassium tantalate $K_{1-x}Li_xTaO_3$, a very complex polar system. In the case of $x < 0.02$, a relaxor or glass-like behavior is realized, while in the concentration higher that $x > 0.02$ a ferroelectric order appears [6]. The results of low temperature linear χ_1’ as well as nonlinear χ_2’and χ_3’electric susceptibility and polarization P measurements of the $K_{1-x}Li_xTaO_3$ are presented. The linear and nonlinear electric response was measured at frequencies $30 \leq f \leq 3\times10^3$ Hz in a gas-flow helium cryostat at temperatures range $4.5 \leq T \leq 300$ K using a self-constructed susceptometer [7]. A discussion concerns the nature of PNRs, mechanism of ferroelectricity and coexistence of relaxor-like and ferroelectric behavior in the solid solution $K_{1-x}Li_xTaO_3$ will be presented.

Acknowledgments
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MULTISCALE LOCAL ORDERING IN UNIAXIAL RELAXOR $Sr_{0.6}Ba_{0.4}Nb_2O_6$

A. Bosak[1], **A. Naberezhnov[2,3]**, S. Vakhrushev[2,3], P. Vanina[3] and S. Borisov[2]

[1]European Synchrotron Radiation Facility, Grenoble, France

[2]Ioffe Institute, St. Petersburg, Russia

[3]Peter the Great Saint-Petersburg Polytechnic University, St. Petersburg, Russia

alex.nabereznov@mail.ioffe.ru

The structure and diffuse scattering in $Sr_{0.6}Ba_{0.4}Nb_2O_6$ (SBN60) single crystal have been studied by X-ray diffraction and neutron scattering in the temperature diapason 290-420 K. At high temperature we have observed the intensive critical scattering in a vicinity of (002) Bragg point. This scattering is described as a sum of two components: the first one corresponds to the Ornstein-Zernike correlation function (lorentzian) and the second input described by lorentzian in square corresponds to the scattering by nanodomains. From temperature dependence of critical scattering we have obtained the temperature dependence of inversed correlation length κ(T), estimated T_C (340.5(12) K) and calculated the critical exponents $\nu = 0.66(2)$ and $\gamma = 1.33(17)$. Below T_C we have observed a "freezing" of the correlation length $\xi = 13(2)$ nm) (Fig.1). It means that below T_C SBN60 does not transform into an ordered state. The distribution of diffuse scattering at room temperature in the planes (H K 0), (H K 1/2), (H K 1), (H K 2), (H 0 L) and (H H L) have been studied by synchrotron radiation. It is shown that there are two different types of diffuse scatterings. For example (Fig. 2a) the intensity distribution near the point (6.31 6.31 0.5) is described by lorentzian in square with two different correlation length: $\xi_{110} \sim 10$ nm and $\xi_{001} \sim 15$ nm. On other hand in the plane of reciprocal space with integer L (Fig. 2b) we have observed the peaks consisted of two components: the fairly narrow elastic Bragg peak and the broad diffuse scattering with lorentzian lineshape. For this scattering we have obtained the second set of correlation lengths: $\xi^{(2)}_{110} \sim 3$ nm along [110] direction and $\xi^{(2)}_{001} \sim 25$ nm along [001].

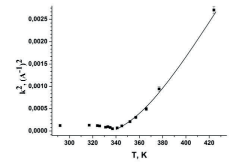

Fig. 1. Temperature dependence of κ.

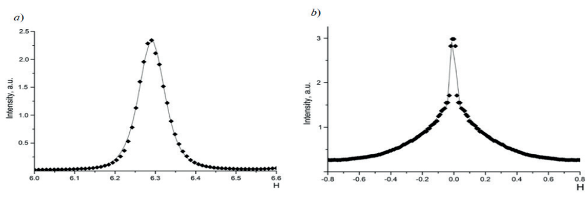

Fig. 2. Lineshapes of peaks in the positions: (a) - (6.31 6.31 0.5), (b) - (5 0 2).

So the study of SBN60 structure at room temperature have revealed the coexistence of two different types of local ordering with different correlation lengths and different forms of correlation functions.

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FLEXIBLE FERROELECTRIC HYBRID FIBERS FOR SOFT BODY SHAPE SENSING

T. Sebastian, T. Lusiola, T. Graule and F. Clemens
Empa - Swiss Federal Laboratories for Materials Science and Technology,
Laboratory for High Performance Ceramics, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland
tutu.sebastian@empa.ch

Piezoelectric fibers are widely investigated for the fabrication of flexible composites especially active fiber composites (AFC's), which consists of unidirectonal axially aligned PZT fibers sandwiched between interdigitated electrodes and embedded in a polymer matrix. However, due to the brittle nature of PZT fibers, maximum strain is limited to 0.3% and cannot be integrated into flexible sensor applications. A good example showing its limitation is while attaching to a curved surface, due to the pre-strain, maximum strain will be significantly reduced [1].

In this contribution, a new approach to achieve flexible one dimensional piezoelectric structures is investigated. Piezoelectric particles incorporated in a polymer matrix and extruded as fiber, 0-3 composite in fibrous form have been studied. Commercially obtained calcined PZT and calcined $BaTiO_3$ powders were used in the unsintered form to obtain flexible soft condensed matter ferroelectric hybrid fibers. The extruded fibers were subjected to investigation for their electromechanical behavior as a function of electric field. The hybrid fibers reached 10% of the maximum strain and polarisation of dense ferroelectric ceramic fibers.

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MIXED VALENCE INFLUENCE ON THE STRUCTURE OF TRANSITION METAL OXIDES

D. Kochnitcharova[1,2], **O. Koleva[1]**, E. Lefterova[1], M. Shipochka[3] and T. Petkova[1]

[1]Section Solid State Electrolytes, Institute of Electrochemistry and Energy systems Acad. Evgeni Budevsky, Bulgarian Academy of Sciences, Sofia, Bulgaria

[2]University of Chemical Technology and Metallurgy, Department of Electrochemistry, Sofia, Bulgaria

[3]Institute of General and Inorganic Chemistry Bulgarian Academy of Sciences, Sofia, Bulgaria

ofeliya.kostadinova@gmail.com

The well-being of the modern society requires continuous increase of the energy demand. This point, combined with the gradual exhaustion of fossil fuels and the fact that their use is accompanied by release of a big amount of noxious gases, requires urgent development of sustainable alternative energy sources and storage. The solid oxide fuel cells (SOFCs) are a forward-looking approach since they can operate reversibly, storing excess renewable electricity in electrolysis mode, and then converting the fuel back to electricity in fuel cell mode [1].

Cost and long-term durability remain significant challenges to more extensive SOFC commercialization. An effective approach to cost reduction is the lowering of the operating temperature without inferring performance losses [2]. Recently an innovative concept, called dual membrane fuel cell (dmFC) was introduced [3-4]. It combines the advantages and bypasses the disadvantages of both SOFC and proton conducting fuel cell (PCFC) in respect to the effect of the water, introducing a separate chamber for its formation and evacuation. The most promising approach in SOFC optimization is the development of new materials with high mixed ionic (protonic and oxide ion) conductivity at lower operating temperatures. A good strategy is the formation of cation-offstoichiometric materials where the charge imbalance caused by the cation non-stoichiometry is compensated by protons. Phosphates are among the materials that receive much attention due to the high thermal conductivity, low melting and softening temperature [5]. Incorporation of transition metal ions (e.g. V) produces new pathways for proton mobility by modification and deformation of the structure.

The present study concerns novel mixed transition oxide $(TiO_2)_x(V_2O_5)_y(P_2O_5)_{100-x-y}$ (x = 5 - 20 mol.% and y = 30 - 70 mol.%) materials. The samples are synthesized and characterized structurally by means of XRD diffraction, IR and XPS spectroscopic techniques. The two of the samples were defined as semicrystalline while the rest were found as completely amorphous. XPS analysis confirms both the transition of V between two valence states: V^{4+} and V^{5+} and different oxygen environment. For all studied samples the IR technique showed presence of VO_5 groups and isolated PO_4^{3-} structural units. The correlation between the structure and the material behaviours are discussed in terms of composuition and valence influence.

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INVITED LECTURE

MULTIFERROELECTRICITY OF CORNER-SHARED NETWORK OF MANGANESE AND OXYGEN

B. Dabrowski[1], O. Chmaissem[1], S. Kolesnik[1], V. Goian[2] and S. Kamba[2]
[1]*Deptment of Physics, Northern Illinois University, DeKalb, IL, USA*
[2]*Institute of Physics, Academy of Sciences of the Czech Republic*
bdabrowski@niu.edu

Multiferroics that exhibit simultaneous ferroelectric and magnetic orders are a topic of current intense investigation both to understand how these two disparate order parameters interact and because of the promising possibility of controlling the magnetic properties electronically and vice versa [1,2]. Type-II or 'improper' multiferroics exhibit strong magnetic-ferroelectric coupling, however, the ferroelectric order parameter is more than two orders-of-magnitude smaller than robust nonmagnetic ferroelectrics such as the prototypical $Ba^{2+}Ti^{4+}O_3$ for which the hybridization of the occupied oxygen p orbitals to the empty Ti *d* orbitals precludes the possibility of magnetic order. Type-I or 'proper' multiferroics with robust displacive-type ferroelectric order are not only rare but also they typically exhibit disparate ordering temperatures and very weak coupling between the order parameters. Recently new promising multiferroics have been discovered with strong coupling. Our work on lightly substituted magnetic $Sr_{1-x}Ba_xMnO_3$ materials synthesized with conventional fabrication techniques up to a maximum x of ~ 0.2 did not reveal ferroelectricity expected for tensile strain elongated Mn-O bonds [3]; however, expanding the Ba concentrations to higher values ($x \geq 0.45$) succeeded in achieving robust ferroelectricity [4]. These ceramics exhibit unique ferroelectricity ($T_F > 300$ K) and G-type antiferromagnetism ($T_N \sim 200$ K) originating exclusively from the Mn^{4+} (d^3) cations.

By advancing elaborate synthesis processes, which are necessary to avoid the more stable hexagonal polymorphs, we were able to prepare and study structural, magnetic and ferroelectric properties [5,6] of highly strained multiferroics for x = 0.4 - 0.45. The classical displacive-type ferroelectric phase occurs with a polarization of several μC/cm^2 when the Mn ions move out of the center of the MnO_6 octahedral units. The Mn spins order below T_N into a simple G-type magnetic structure while the ferroelectric order decreases dramatically demonstrating that the two order parameters are strongly coupled. A spin gap of 4.6(5) meV and the magnon density of states peaking at 43 meV characterize the ground state spin dynamics. The ferroelectric phase transition has a signature of a crossover from displacive to order-disorder type. The phonons are coupled with a central mode but contribution to ε' is rather small. The lowest-frequency polar phonons are overdamped above T_N and they exhibit pronounced softening on heating towards T_C.

We have recently extended investigation of manganites to the Ti-substituted $Sr_{1-x}Ba_xMn_{1-y}Ti_yO_3$ system for which ferroelectricity above 400 K and structural distortions characterizing polarization significantly exceeding that of the classical titanates were observed. The T_N decreases to below 200 K and the suppression of ferroelectricity below T_N is reduced, i.e., we achieved displacive-type multiferroic with large spontaneous polarization. I will describe unique properties of these materials.

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DEMONSTRATION OF SPIN-PHONON COUPLING IN INFRARED, THz SPECTRA AND MICROWAVE PERMITTIVITY OF $Sr_{1-x}Ba_xMn_{1-y}Ti_yO_3$ CERAMICS AND $Sr_{0.6}Ba_{0.4}MnO_3$ THIN FILMS

V. Goian[1], V. Bovtun[1], C. Kaldec[1], F. Kadlec[1], M. Kempa[1], D. Nuzhnyy[1], B. Dabrowsky[2], E. Langenberg[3], J. Pardo[3] and S. Kamba[1]

[1]*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*

[2]*Department of Physics, Northern Illinois University, DeKalb, IL, USA*

[3]*Institute of Nanoscience of Aragón, University of Zaragoza, Spain*

goian@fzu.cz

Recent first principles calculations predicted a large spin-phonon coupling in various manganites, chromides and ferrites with perovskite structure [1], so these materials can theoretically become new multiferroics under strain or with appropriate doping.

In this work, we will focus on $Sr_{1-x}Ba_xMn_{1-y}Ti_yO_3$ (x = 0.5, 0.6 and y = 0.06, 0.1) perovskites where we will demonstrate phonon anomalies near ferroelectric and antiferromagnetic phase transitions. Pure $SrMnO_3$ crystallizes in cubic perovskite $Pm\overline{3}m$ crystal structure and exhibits magnetic phase transition to antiferromagnetic G-type phase near 230 K [2]. Close to this temperature 23% hardening of the lowest-frequency phonon was revealed in the IR spectra due to spin-phonon coupling [3]. Although $SrMnO_3$ is paraelectric down to liquid He temperatures, recent first principles calculations predicted that system can become ferroelectric and even ferromagnetic under a biaxial strain [4]. The strain-induced ferroelectricity was not yet confirmed experimentally in $SrMnO_3$, but Sakai et al. [5] expanded $SrMnO_3$ lattice by Ba doping and successfully induced ferroelectricity in $Sr_{1-x}Ba_xMnO_3$ ($x \approx 0.45$) crystals with $T_C \approx 400$ K and Néel temperature $T_N \approx 200$ K. Important fact is that in this case the strong ferroelectricity (P_S = 13 μC/cm^2) is driven by displacement of magnetic Mn^{4+} cations, so exceptionally strong magnetoelectric coupling is expected.

Unfortunately, the conductivity influences the permittivity in MW and even THz range of $Sr_{0.6}Ba_{0.4}MnO_3$ ceramics. Hopping conductivity can be strongly reduced by Ti doping. For that reason we investigated $Sr_{1-x}Ba_xMn_{1-y}Ti_yO_3$ where y = 0.06 and 0.1 and x = 0.6 and 0.5. Microwave permittivity and conductivity is still influenced by hopping conductivity, but permittivity of $Sr_{0.4}Ba_{0.6}Mn_{0.94}Ti_{0.06}O_3$ exhibits a peak at ferroelectric phase transition near 400 K. Ferroelectric phase transition is seen as well in phonon permittivity obtained from the fits of THz and IR reflectivity spectra. Spin-phonon coupling is manifested by the jump of THz permittivity near T_N. THz permittivity of $Sr_{0.4}Ba_{0.6}Mn_{0.94}Ti_{0.06}O_3$ ceramics was measured in external magnetic field up to 7 T. No change was surprisingly detected. It means, the magnetodielectric effect is under resolution of our THz spectrometer despite of huge spin-phonon coupling present in investigated ceramics.

In $Sr_{0.6}Ba_{0.4}MnO_3$ thin film deposited on LSAT and $TbScO_3$ no ferroelectric phase transition was detected. Spin-phonon coupling was revealed near Neel temperature only in the IR spectra of $Sr_{0.6}Ba_{0.4}MnO_3$ film grown on LSAT.

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ROLE OF La AND Mn SUBSTITUTION ON STRUCTURE AND ELECTRIC PROPERTIES OF BISMUTH FERRITE

T.T. Carvalho[1], J.R.A. Fernandes[2], P.B. Tavares[3], J. Agostinho Moreira[1] and A. Almeida[1]

[1]*IFIMUP and IN, Physics & Astronomy Dep., Faculty of Sciences, University of Porto, R. Campo Alegre, 687, 4169-007 Porto, Portugal*

[2]*INESC TEC and Physics Departament, University of Trás-os-Montes e Alto Douro, 5001-801 Vila Real, Portugal*

[3]*CQVR and Chemistry Department, University of Trás-os-Montes and Alto Douro, 5001-801 Vila Real, Portugal*

ttranchete@fc.up.pt

Bismuth ferrite ($BiFeO_3$) is a perovskite material, rich in properties and very attractive in the design of new multifunctional devices within spintronics [1]. In this system the ferroelectric behavior is related to the stereochemical activity of the Bi^{3+} lone pairs. A recent study combines symmetry arguments and first-principles calculations to explore the connection between structural distortions and ferroelectricity in the perovskite family of materials [2].

Some drawbacks limit the electronic applications such as low remnant polarization and weak magnetoelectric coupling [3]. Different attempts have been made in order to overcome this limitation such as the substitution of A-site and/or B-site of the perovskite lattice that improve electric behavior and enhance magnetic properties.

Co-substitutions with lanthanum and manganese have been reported has an effective way to decrease leakage current density and allow the presence of ferromagnetic behavior [4]. However it is necessary to understand the role of each dopant on co-doped samples in order to “design” a multiferroic system with improved electric and magnetic properties.

In this work we study the role of each dopant (La and Mn) on structural and magnetic properties of the BFO. Our study focus on the low content co-doped samples, the 10% lanthanum content and 1 - 10% of manganese content.

Lanthanum partial substitution alone or on codoping promotes the reduction of secondary phases. Simultaneous substitution with lanthanum and manganese promotes a decrease of dielectric losses.

Detailed analyses of Raman spectra reveal A site disorder accompanied by a change in oxygen octahedral in BLFM samples.

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DEVELOPMENT OF LANDAU POTENTIAL FOR $BiFeO_3$

P. Marton[1,2], A. Klíč[1], M. Paściak[1] and J. Hlinka[1]
[1]*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*
[2]*Institute of Mechatronics and Computer Engineering, Faculty of Mechatronics, Informatics, and Interdisciplinary studies, Technical University of Liberec, Liberec, Czech Republic*
marton@fzu.cz

$BiFeO_3$ is an extremely interesting multiferroic material with wide potential applications. In its rhombohedral ground-state it has a large ferroelectric polarization of about 0.7 C/m^2, which is accompanied by strong shifts and tilts of oxygen octahedra. It is known from experiments and theory that the ferroelectric domain walls in $BiFeO_3$ have interesting properties such as elevated electric conductivity and others. Nevertheless, a trustworthy phenomenological model which would allow to take important aspects of the local properties (ferroelectric polarization, oxygen tilts, deformation) into account and yet enable to study properties of domain walls of different types and their interaction or even its dynamics is, to our opinion, still missing, although there are already several publications of such potentials [1-3]. For this sake we present here our attempt to develop the Landau-type potential for $BiFeO_3$ based on first-principles calculation. The obtained parametrization of the Landau potential is compared with those in the aforementioned references.

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FIRST-PRINCIPLES STUDY OF HIGH-PRESSURE PHASES OF $BiGaO_3$

J. Kaczkowski
Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland
kaczkowski@ifmpan.poznan.pl

The first-principles total energy calculations of $BiGaO_3$ in different crystal phases under pressure up to 20 GPa have been performed within generalized gradient approximation (GGA). The calculations were done within projector-augmented wave method as implemented in VASP. The structural phase transition appears at 3.5 GPa from pyroxene-like structure (paraelectric, Pcca space group) to perovskite-like structure (ferroelectric, space group) [1]. This is consistent with experimental results [2]. At 5 GPa coexistance of three ferroelectric phases (i.e. monoclinic Cm, tetragonal P4mm, and rhombohedral R3c) have been found. At 7 GPa phase transition from rhombohedral R3c to orthorhombic Pnma phase have been predicted. Calculated spontaneous polarization of ferroelectric phases are: 130 μC/cm^2 for Cm, 90 μC/cm^2 for R3c, and 124 μC/cm^2 for P4mm.

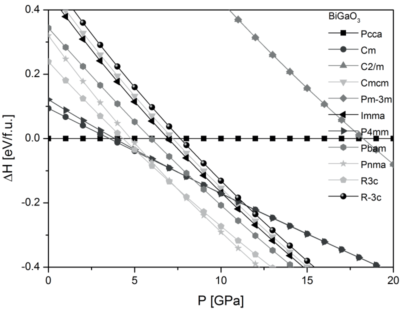

Fig. 1. Calculated enthalpy as a function of pressure for different phases of $BiGaO_3$.

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INVITED LECTURE

SOFT MODES IN IMPROPER FERROELECTRICS AND MULTIFERROICS

S. Kamba
Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
kamba@fzu.cz

In proper ferroelectrics, the large dielectric anomaly in permittivity ε'(T) occurring at the Curie temperature T_C is caused by softening of a polar optical phonon or by slowing down of a microwave dielectric relaxation. Such soft modes drive ferroelectric phase transitions in $BaTiO_3$ or the type-I multiferroics like $PbFe_{0.5}Nb_{0.5}O_3$ or strained $EuTiO_3$. In improper ferroelectrics a multiplication of unit cell occurs and only a small change of slope in ε'(T) appears at T_C because ferroelectric soft mode activates in IR spectra only below T_C. This behaviour we will demonstrate on $BaMnO_3$ and $BiFeO_3$ [1]. In the spin-order induced ferroelectrics (i.e. type-II multiferroelectrics), only small dielectric anomalies are observed at ferroelectric T_C, because these materials belong to improper or pseudoproper ferroelectrics (i.e., the order parameter is some other quantity than polarization). For the type-II multiferroics with noncollinear magnetic structure, Katsura, Balatsky and Nagaosa predicted already in 2007 that soft spin waves hybridized with the electric polarization should drive the ferroelectric phase transitions [2]. These spin waves can be called electromagnons, because they contribute to both dielectric permittivity and magnetic permeability. Only last year, Niermann et al. [2] confirmed this prediction, having discovered a critical slowing down of a Drude-like dielectric relaxation near the multiferroic phase transition in $MnWO_4$. The relaxation was observed in the microwave dielectric spectra only within 0.2 K above T_C, because at higher temperatures the relaxation frequency hardens above 10 GHz and its dielectric strength becomes negligible. This excitation was interpreted as the soft electromagnon which drives the ferroelectric phase transition [3].

Similar small and narrow dielectric peaks at T_C are known from most spin-induced ferroelectrics, but they were never investigated using microwave dielectric spectroscopy in the vicinity of T_C. Nevertheless, electromagnons were observed for most multiferroics with spiral magnetic structures in their THz spectra. Thus, their frequencies are two or three orders of magnitude higher and we propose, based on analogy with phonons in structurally modulated crystals, that they correspond to the amplitudon component of the spin wave, whereas the soft microwave component is a phason component of the electromagnon activated by the inverse Dzyaloshinskii-Moriya interaction. We will demonstrate this behaviour in $(Ba_xSr_{1-x})_3Co_2Fe_{24}O_{41}$ crystallizing in the Z-type hexaferrite structure.

Another type of multiferroics with improper ferroelectric phase transitions is represented by orbital-order driven ferroelectrics with the Jahn-Teller transitions. GaV_4S_8 belong to this family and it undergoes the ferroelectric and magnetic phase transitions at 44 K and 12.7 K. In its paraelectric phase, an overdamped soft mode arising from coupled orbital and polar fluctuations was detected in the THz region and its relaxation frequency drops by five orders of magnitude at the first order ferroelectric phase transition. Another small hardening was detected at the magnetic phase transition, when Skyrmion lattice appears [4].

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KEY LECTURE

POLARIZED RAMAN SCATTERING ON BISMUTH FERRITE

J. Pokorný, F. Borodavka and J. Hlinka
Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
pokorny@fzu.cz

Bismuth ferrite ($BiFeO_3$) is a prototypical multiferroic system with a coexistence of ferroelectric and magnetic order at room temperature: it is ferroelectric up to $T_C \sim 1100$ K and antiferromagnetic up to $T_N \sim 640$ K. At room temperature, $BiFeO_3$ exhibits a rhombohedrally distorted perovskite structure with *R*3*c* symmetry. Its application potential is extended by the possibility of preparing various solid solutions [1].

Characterization of polar phonon modes is essential for understanding dielectric and electromechanical behaviour. In our previous work [2], we have determined the complete spectrum of $BiFeO_3$ polar modes. The experiment also yielded a full directional dispersion of oblique mode. Morover, we have realized that Raman back-scattering by the oblique modes can be used to determine the orientation of the rhombohedral axis with respect to the sample surface. Our mode assignment [2] has been confirmed in several recent works [3,4].

Here we describe the polarization anisotropy of Raman scattering in $BiFeO_3$. Among others, we show how this information can be employed to complement the information from the directional dispersion when analyzing grain interfaces and ferroelastic domain walls in this material.

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HIGH TEMPERATURE DIELECTRIC RESPONSE IN SIZE SCALED $BiFeO_3$

K. Chybczyńska, E. Markiewicz, B. Hilczer and B. Andrzejewski
Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
katarzyna.chybczynska@ifmpan.poznan.pl

Ball-like flowers of $BiFeO_3$ (BFO) with petals/crystallites the thickness of which can be controlled within 100 - 300 nm were obtained by microwave assisted hydrothermal synthesis. Below 450 K the dielectric response of ceramics made of the crystallites with mean thickness <D> = 160 nm and <D> = 260 nm was found to be similar to that of nanoceramics prepared from mechanoechemically synthesized BFO [1]. A considerable increase in the dielectric permittivity observed above 450 K was found to be correlated with the temperature variation of the electric conductivity. The dc contribution to the conductivity was found to be characterized by activation energy of 1.73 eV for ceramics with <D> = 160 nm and 1.52 eV for the ceramics with <D> = 260 nm which is higher than that for other $BiFeO_3$ nanoceramics (1.1 eV). The increase in the activation energy we relate to interactions between oxygen vacancies and size scaled ferroelectric/ferroelastic domain walls [2], which in $BiFeO_3$ are associated with electrostatic potential steps [3]. We calculated that in the samples with mean crystallite thickness of 160 nm the distance between domain walls is ~ 30% shorter than that in BFO with mean crystallite thickness of 260 nm [4]. Thus the activation energy of dc conductivity of BFO ceramics with thinner crystallites is higher since the oxygen vacancies are pinned by higher density of ferroelectric/ferroelastic domain walls, which in BFO are associated with potential step of 0.15 - 0.18 eV.

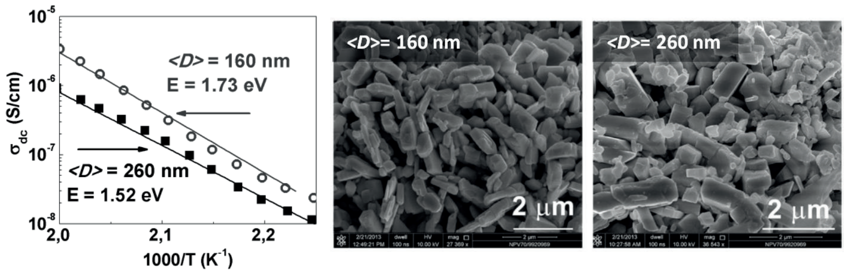

Fig. 1. High-temperature σ_{dc} conductivity versus reciprocal temperature (left), SEM images of BFO powder with crystallites of mean thickness <D> = 160 nm and <D> = 260 nm.

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SYNTHESIS AND DIELECTRIC INVESTIGATIONS OF $BaTi_4O_9$ OBTAINED BY SOFT CHEMISTRY ROUTE

A. Wypych-Puszkarz, I. Bobowska, A. Opasińska, A. Wrzesińska and J. Ulański
Lodz University of Technology, Department of Molecular Physics,
Faculty of Chemistry, Żeromskiego 116, 90-924 Lodz, Poland
aleksandra.wypych@p.lodz.pl

Materials with high dielectric permittivity are widely explored due to their importance in electronic components such as capacitors, gate dielectrics, memories or power-storage devices. Barium titanate in a form of $BaTi_4O_9$ is TiO_2 rich compound in BaO-TiO_2 family, which is characterized by a high dielectric constant (almost 40), good quality factor and low value of temperature coefficient [1]. Nowadays, the trend of development is a miniaturization of components and thin layers synthesis so that ceramics obtained by classical solid state route do not follow the actual requirements. From this reason many different methods including e.g. chemical bath deposition, co-precipitation or sol-gel processes are applied and products of their synthesis are carefully explored. These methods are classified as soft or wet chemistry routes and have considerable advantages over conventional solid-state reactions, such as: better compositional control, nano-sized precursor powders and resulting from it lower crystallization temperature, avoiding the grinding step in synthesis procedure and possible contamination.

In this work barium titanate precursor was obtained from reaction of aqueous solution of titania nanosheets, used as a source of titanium [2], and barium salt. Mixing both substrates in solution allows their intimate blending and produces nanosized organic-inorganic precursor of barium titanate being the precipitate of this reaction. The obtained barium titanate precursor were subjected to step sintering and final products were investigated by: X-ray diffraction analysis, Raman and broadband dielectric spectroscopies. Dielectric properties and microstructure of ceramic grains, as seen by scanning electron microscopy, were carefully examined parallel to applied step sintering. It was found that with an increase of sintering temperature the apparent density and dielectric constant (ε) of ceramic pellets increase. The rapid contraction of calcinated sample was found between temperature of 1000 °C and 1050 °C. The dielectric constant of pellet was found to be equal 30 and 33, respectively. Further calcination, above 1100 °C, leads to the increase of dielectric constant ($\varepsilon = 38 \div 39$) that results from an increase of ceramic pellet's density and transformation of compound to titanate of different stoichiometry, i.e. $Ba_2Ti_9O_{20}$.

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Acknowledgements

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INVITED LECTURE

NEUTRON SCATTERING IN MULTIFERROICS: THE EXAMPLE OF $YMnO_3$

Ch. Simon
Institut Laue Langevin, Grenoble, France
simon@ill.fr

Multiferroics are for already a decade subject of intense activity, related to its possible applications in magnetic recording. We performed different measurements, associated with Landau theory and symmetry analysis, in order to clarify the situation of the $YMnO_3$ system, a classical example of type I multiferroics. We found that the only magnetic group compatible with all experimental data (neutron scattering, magnetization, polarization, dielectric constant, second harmonic generation) is the P6(3)' group. In this group a small ferromagnetic component along c is induced by the Dzyaloshinskii-Moriya interaction, and observed here in magnetization measurements. We found that the ferromagnetic and antiferromagnetic components can only be switched simultaneously, while the magnetic orders are functions of the polarization square and therefore insensitive to its sign. This paper also proposes the direct calculation of the microscopic contributions to the magneto-electric coupling, using ab initio methods. The electrostrictive and the Dzyaloshinskii-Moriya contributions were evaluated individually. In $YMnO_3$ the Dzyaloshinskii-Moriya contribution to the magneto-electric effect is three orders of magnitude weaker than the electrostrictive contribution. These effects however, remain quite small. The linear magneto-electric tensor is null due to the inter-layer symmetry operations.

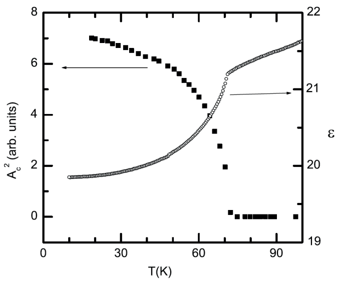

Fig. 1. Temperature dependence of the dielectric constant (right) compared to the amplitude of the 100 antiferromagnetic peak of neutron diffraction (left).

Charles Simon thanks all his co-authors of previous publications on this subject and in particular Kiran Singh, Marie-Bernadette Lepetit, Natalia Bellido, Stephane Pailhes, Julien Varignon, A. De Muer, I. Gélard, C. Dubourdieu, G. Nenert.

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KEY LECTURE

INVESTIGATIONS OF PHASE TRANSITIONS ON THE NANOMETER SCALE BY NEUTRON SPIN ECHO SPECTROSCOPY

P. Fouquet
Institut Laue-Langevin, CS 20156, 38042 Grenoble Cedex 9, France
fouquet@ill.fr

Phase transitions in materials are often accompanied by dramatic changes of the mobility of the atoms or the spin system. Diffusivities, for example, will change by several orders of magnitude within a few degrees of the transition temperature. This makes the dynamics at phase transitions at the same time highly exciting and experimentally challenging.

In this presentation, we will discuss merits and recent progress of a neutron spectroscopy technique that is particularly well adapted to the study of dynamics at phase transitions because of its unique dynamic range: neutron spin echo spectroscopy (NSE). NSE delivers space-time correlation functions for the atomic positions and the spin system over six orders of magnitude from picoseconds to microseconds (see Fig. 1). With this dynamic window, we have recently studied phase transitions in spin-glasses [1], in multi-ferroics [2] and in structural glasses [3] as well as on surfaces [4]. We will present some of the most intriguing examples from recent years. Finally, we will use this opportunity to present the recent developments of the spin-echo spectrometers IN15 and WASP at the ILL, which will allow us to gain several orders of magnitude in signal and resolution.

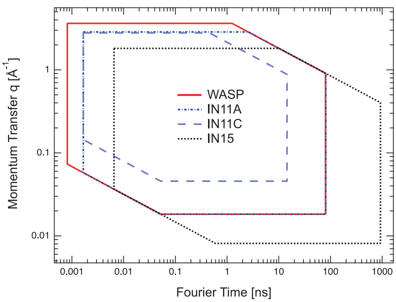

Fig. 1. Dynamic window of the neutron spin-echo spectrometers at ILL.

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SOFTENING OF ELASTIC CONSTANTS IN RELAXOR PZN-8% PT BY INELASTIC NEUTRON SCATTERING

M. Kempa[1], P. Ondrejkovic[1], J. Kulda[2] and J. Hlinka[1]

[1]*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*

[2]*Institut Laue-Langevin,Grenoble, France*

kempa@fzu.cz

Relaxor ferroelectrics are well known, among all, for very high piezoelectric coefficients. There are indications that these piezoelectric properties are related to giant softening of elastic constants, caused by coupling between acoustic and relaxation modes [1]. The elastic constants exhibit their minimum values around the phase transition (or the freezing temperature) which is most likely connected with polar nanoscopic fluctuations in the material. In the case of the single crystal of $Pb(Zn_{1/3}Nb_{2/3})O_3$ with 4.5%$PbTiO_3$ (PZN-4.5%PT), the C_{11}-C_{12} elastic constant was reported to change by 75% on cooling from the paraelectric phase [2]. The technique employed therein, resonant ultrasound spectroscopy (RUS), operates at frequencies below ~1 MHz, which from the viewpoint of phonon dispersion curves means practically in the centre of the Brillouin zone (BZ).

Several inelastic neutron scattering studies in other relaxors reported only weak softening of acoustic branches [e.g. 3,4], however in the region far from the BZ centre (f ~ 1 THz, q ~ 0.1 r.l.u.). In this contribution we will present temperature dependence of transverse acoustic frequencies, corresponding to C_{11}-C_{12}, measured on the morphotropic-phase-boundary single crystal of PZN-8%PT. The data were collected on the newly build cold three axis spectrometer ThALES (ILL Grenoble) which allows to get closer to the BZ centre (f <~ 200 GHz, q ~ 0.03 r.l.u.). The results, indicating rather moderate softening, are discussed together with previously published data with respect to lattice dynamics and anharmonic effects.

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UNIVERSAL FEATURES OF CONDUCTIVITY SPECTRA IN SOME CRYSTALLINE PROTONIC CONDUCTORS

P. Ławniczak, M. Zdanowska-Frączek, A. Pawłowski and Cz. Pawlaczyk
Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
lawniczak@ifmpan.poznan.pl

One of the interesting features of most common disordered ion conductors, independently of differences in their structure and type of ionic charge carriers, is universal frequency response of conductivity spectra [1,2]. The first universality is a characteristic frequency dependence of the real part of electric conductivity. Using a proper scalling method, it is possible to rescale such dependencies measured for various temperatures to single curve. It refers to the thermally activated hopping mechanism of ionic migration in microscopic scale. The second universality, often called Nearly Constant Loss, occurs at sufficiently low temperatures of high frequencies, where translational movements of ions do not contribute to dielectric loss.

Our previous results show that similar universal response can be observed at crystalline, hydrogen bonded proton conductors [3,4]. Investigated material, benzimidazolium azelate, belongs to the family of materials comprised of organic dicarboxylic acids and heterocyclic molecules (i.e. imidazole, 1,2,4-triazole, benzimidazole). They have a layer type structure with hydrogen bond network between acid and heterocyclic molecules, which clearly enables proton migration in layers [4,5].

This contribution is dedicated to present studies of universal conductivity response in crystalline protonic conductors, which undergoes a phase transitions from low to higher, superprotonic, conductivity phase. The dynamics of proton migration changes significantly at the transition temperature T_s. The object of invastigations are well-known superprotonic crystals, $(NH_4)_3H(SO_4)_2$ and $Rb_3H(SeO_4)_2$. Former crystal undergoes superprotonic phase transition at ~413 K, while the latter undergoes phase transitions at ~453 K. The measurements were made using impedance spectroscopy method in the frequency range 10 Hz - 3 GHz.

Comparison of conductivity spectra of superprotonic conductors (with superionic phase transition) and "normal" protonic conductors (without phase transition) show similar universal features as common solid state ionic conductors.

Acknowledgment
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SINGLE-PARTICLE AND COLLECTIVE STATES OF WATER MOLECULES IN THE MATRIX OF BERYL CRYSTAL LATTICE: EXPERIMENT AND THEORY

M. Belyanchikov[1,2], S. Tretiak[9], E. Zhukova[1,2,3], V. Thomas[5], D. Fursenko[5], P. Thomas[7,8], M. Savinov[6], C. Kadlec[6], F. Kadlec[6], J. Petzelt[6], M. Dressel[3] and B. Gorshunov[1,2,3]

[1]*Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, 141700 Russia*

[2]*A.M. Prokhorov General Physics Institute, RAS, Moscow, 119991 Russia*

[3]*1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany*

[4]*Faculty of Physics, Southern Federal University, 344090 Rostov-on-Don, Russia*

[5]*Institute of Geology and Mineralogy, RAS, 630090 Novosibirsk, Russia*

[6]*Institute of Physics AS CR, Na Slovance 2, 18221 Praha 8, Czech Republic*

[7]*National Research University Higher School of Economics, 101000, Moscow, Russia*

[8]*Independent University of Moscow, 119002, Moscow, Russia*

[9]*Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, USA*

belyanchikov@phystech.edu

An array of separate water molecules that are located within a periodical matrix of sub-nanometer-sized pores formed by the ions of hexagonal crystal lattice of a beryl is an excellent system for spectroscopic investigations of single-particle and collective states of dipole-dipole coupled H_2O molecules. Here caged water molecules are trapped in either of two orientations of their dipoles: type I or II, which refer to directions perpendicular to or parallel with the hexagonal crystallographic c-axis, respectively. Using dielectric spectroscopy, we have detected, on the background of phonon lines, a rich and strongly anisotropic set of absorption resonances caused exclusively by the water subsystem [1-3]. The resonance absorptions in the infrared range were preliminarily assigned to librational and translational modes of caged H_2O molecules. The origin of the temperature unstable excitation at terahertz frequencies remained unclear. In this contribution, we discuss the nature of the observed absorption spectra. By using the density functional theory (DFT) approach, we demonstrate, on a quantitative level, that the infrared resonances are related to librational and rotational motions of separate type-I and type-II water molecules. We further extend the mean-field model of Nakajima and Naya [4] to the case of a 6-well potential experienced by the rotating/librating dipoles. Based on the developed model, we associate the terahertz excitation with the ferroelectric soft mode that is connected with the onset of incipient ferroelectricity within the network of caged water molecules.

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MAGNETOELECTRIC MECHANISMS OF SLIGHTLY B-site DOPED $TbMnO_3$

R. Vilarinho[1], E. Queiros[2], D.J. Passos[1], D.A. Mota[1], P.B. Tavares[2], M. Mihalik jr.[3], M. Zentkova[3], M. Mihalik[3], A. Almeida[1] and J. Agostinho Moreira[1]

[1]*IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Physics and Astronomy Department of Faculty of Sciences of University of Porto, Porto, Portugal*

[2]*Centro de Química, Universidade de Tras-os-Montes e Alto Douro, Vila Real, Portugal*

[3]*Institute of Experimental Physics, SAS, Watsonova 47, 040 01 Kosice, Slovakia*

rvsilva@fc.up.pt

$TbMnO_3$ is a well-known multiferroic. Its phase sequence can be summarized as follows: At T_N = 41 K, it undergoes a phase transition into a incommensurate antiferromagnetic phase, with a longitudinal spin density wave propagating along the *a*-axis, using Pbnm. Below Tlock = 27 K, a commensurate cycloidal magnetic order in the *bc*-plane stabilizes, and a spontaneous polarization emerges along the *c*-axis, according to the Dzyaloshinskii-Moriya mechanism [1]. At T_1 = 7 K, the Tb^{3+} spins order independently from the Mn^{3+} ones [1].

Recently it has been shown that the inclusion of magnetic non-active Jahn-Teller cations (Co^{3+}, Cr^{3+}, Fe^{3+}) in the B-site of $TbMnO_3$, even in small concentrations ($x < 0.1$), induces substantial changes of its physical properties [2]. These studies however have been mainly focused on the effect on the magnetism, and only few on the ferroelectricity and magnetoelectric coupling, which still deserve attention since the interpretation of the experimental results through the role played by the eg-orbital electrons is controversial [2,3].

This work aims at unraveling the effect of Fe^{3+} substitution, up to x = 0.05, in the magnetic, ferroelectric and magnetoelectric properties of the $TbMn_{1-x}Fe_xO_3$ system as a function of both temperature and applied magnetic fields, up to 9 T. A strong decrease of the polarization with increasing Fe^{3+} substitution is observed. However, within the stability range, a significant increase of the magnetic sensitivity of the polarization is obtained. Above 4% of Fe-concentration, a non-polar, weak ferromagnetic antiferromagnetic phase emerges, in good agreement with the predictions of the Dzyaloshinskii-Moriya model. The results reveal the crucial effect of Fe^{3+} substitution, and are discussed in the scope of available theoretical framework, understood as a consequence of the competition between ferromagnetic and antiferromagnetic interactions, very sensitive to both local fields and distortions [3].

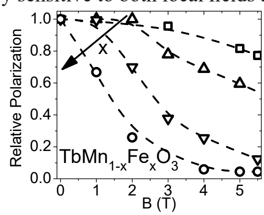

Fig. 1. Relative polarization of $TbMn_{1-x}Fe_xO_3$, $0 \le x \le 0.05$, as a function of magnetic field.

We acknowledge the support of the projects Norte-070124-FEDER-000070 and PTDC/FIS-NAN/0533/2012.

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MACROSCOPIC LAMELLAR HETEROPHASE PATTERN IN $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ SINGLE CRYSTALS

I. Rafalovskyi[1], M. Guennou[1,2], I. Gregora[1] and J. Hlinka[1]
[1]*Institute of Physics, The Czech Academy of Sciences, Na Slovance 2, 182 21 Prague 8, Czech Republic*
[2]*Materials Research and Technology Department, Luxembourg Institute of Science and Technology, 41 rue du Brill, L-4422 Belvaux, Luxembourg*
rafalov@fzu.cz

Crystalline solid solution $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) is a promising material for electromechanical sensor and actuator applications [1-3]. Here we describe lamellar heterostructures, observed in PMN-xPT single crystals with x = 0.32. Such structures can be obtained while cooling under bias electric field applied along pseudocubic direction, and then zero-field heating to the temperature close to the depoling temperature TRT. The same lamellar configuration can be obtained even at ambient conditions. These structures were investigated by polarized micro-Raman measurements in details, showing that these lamellar structures are composed of tetragonal-like and rhombohedral-like layers [4].

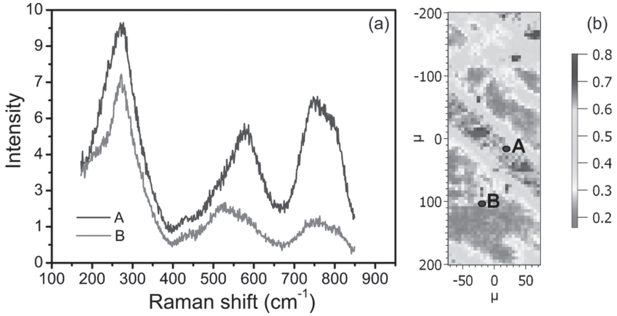

Fig. 1. Micro-Raman study of the stripe pattern of a PMN-0.32PT single crystal prepared by ZFHaFC process. (a) Cross-polarized [*z(xy)z*] Raman spectrum of a PMN-0.32PT single crystal taken from spots (A) and (B) within dark and light stripes, respectively. (b) Map of the I780/I270 ratio of the cross-polarized Raman scattering intensities recorded at 780 and 270 cm^{-1} reveals the stripe pattern. (The edges of the imaged area areparallel to the pseudocubic crystal axes and to the sample edges as well.)

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ESTER DERIVATIVES OF 4-PENTYL-4- HYDROXYAZOBENZENE-SYNTHESIS AND CHARACTERIZATION

I. Niezgoda[1], D. Pociecha[2] and Z. Galewski[1]
[1]*Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland*
[2]*Faculty of Chemistry, Warsaw University, Warsaw, Poland*
izabela.niezgoda@chem.uni.wroc.pl

Azobenzene derivatives are very interesting materials because of their photosensitivity [1] but also due to possible rich liquid-crystalline polymorphism [2]. Because of the above described optical properties azo compounds can be applied in many branches of the modern technologies [3].

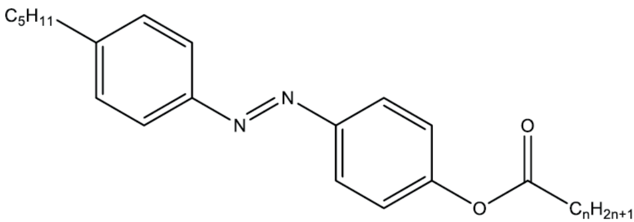

Fig. 1. Chemical structure of synthesized and investigated homologues series of azobenzene derivatives.

Aim of this research was synthesis and characterization of full homologues series (which consist of 19 compounds) of 4-pentyl-4-hydroxyazobenzene alkanotes. During the characterization process liquid crystalline and photoizomerization studies were conducted. Synthesized materials exhibit very interesting and rich mesomorphism, which was investigated by the use of POM (polarized optical microscopy), TOA (thermos-optical analysis), DSC (differential scanning calorimetry) and XRD (X-Ray diffraction) studies. Moreover, the kinetics of the trans-cis trans isomerization process was explored by the use of UV-Vis spectroscopy. Obtained results gave an important insight to the correlation between the length of the ester chain and observed properties of our materials.

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MAGNETOELECTRIC SPIN EXCITATIONS IN MULTIFERROIC Ni_3TeO_6

S. Skiadopoulou[1], C. Kadlec[1], F. Kadlec[1], J. Prokleška[2], F. Borodavka[1], M. Savinov[1], M. Retuerto[3], Zheng Deng[3], M. Greenblatt[3] and S. Kamba[1]

[1] *Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic*

[2] *Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic*

[3] *Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, USA*

stella@fzu.cz

Ni_3TeO_6 presents a collinear antiferromagnetic order below 52 K, giving rise to spin-induced-ferroelectricity. Among the spin-order driven multiferroics, only Ni_3TeO_6 exhibits non-hysteretic colossal magnetoelectric effect near 8.5 T and 52 T, where spin-flop and metamagnetic phase transitions occur, respectively [1,2]. The lack of hysteretic behavior in the magnetic field dependence of magnetization and dielectric constant precludes losses for a series of magnetoelectric applications.

In the current work, we investigated the spin and lattice excitations of Ni_3TeO_6 ceramics and single crystals. Infrared, time-domain THz and Raman spectroscopy experiments were conducted for a temperature range of 5 to 300 K. Time-domain THz spectroscopy at external magnetic field was carried out at selected temperatures below and close to the antiferromagnetic phase transition. The THz spectra revealed dynamic magnetoelectric coupling, i.e. tuning of THz spectra with magnetic field. Simultaneous infrared and Raman active spin excitations correspond to electromagnons, highly sensitive on magnetic field (Fig. 1).

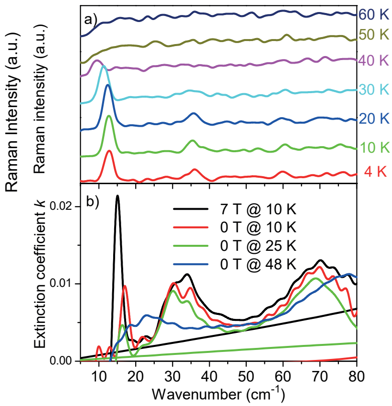

Fig. 1. (a) Raman and (b) THz spectra of Ni_3TeO_6 ceramics revealing two simultaneously detected spin excitations.

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KINETICS OF PHASE TRANSITION IN $(NH_4)_4H_2(SeO_4)_3$

Ł. Lindner[1], M. Zdanowska-Frączek[1], Z. Czapla[2] and Z.J. Frączek[1]
[1]*Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland*
[2]*Department of Physics, Opole University of Technology, Opole, Poland*
lindner@ifmpan.poznan.pl

Hydrogen sulfate and selenate family crystals with general formula $M_xH_y(XO_4)_{(x+y)/2}$ (M=K, Rb, Cs, NH_4, X=S, Se) exhibit high protonic conductivity in superprotonic phase. This characteristic phase transition is accompanied by an increase in the conductivity by a few (1-3) orders of magnitude. One of the reasons for the appearance of superionic phases is the formation of a disordered hydrogen-bond network in these structures. We carried out research on better understanding of the mechanism that control the formation of high conductivity phases.

This study is devoted to a deeper understanding of the factors that control the formation of the high conductive phase in the $(NH_4)_4H_2(SeO_4)_3$ proton conductor. The kinetics study results of pressure induced transformation to superionic phase in $(NH_4)_4H_2(SeO_4)_3$ crystal are also presented. The crystal undergoes superionic phase transition at T_s = 378 K.

The effect of hydrostatic pressure on proton conductivity in $(NH_4)_4H_2(SeO_4)_3$ superionic crystal has been studied at a wide temperature range and different isobaric conditions by means of impedance spectroscopy method. The obtained pressure-temperature phase diagram up to 550 MPa is linear with increasing pressure.

At ambient pressure phase transition from low conductivity phase with space group P-1 and superprotonic $R\bar{3}m$ exist at T_s = 378 K. Impedance spectroscopy studies of electrical conductivity versus time were performed in a single $(NH_4)_4H_2(SeO_4)_3$ crystal at different pressure values up to 360 MPa and temperatures T = 347.3 K and 352.3 K. It was found that the conductivity value increases when the pressure increases and the activation volumes determined from the pressure dependence of the electrical conductivity are always negative. The sluggish solid-solid transformation from low conducting to superionic phase was induced at 302 MPa pressure and T = 352.3 K temperature. It has been established that the kinetics of this transformation can be described by the Avrami model with the effective Avrami index value of about 4 which corresponds to the classical value associated with homogeneous nucleation and three-dimensional growth of a new phase.

INVITED LECTURE

SELF-ASSEMBLED PEPTIDES: STRUCTURE, PROPERTIES, APPLICATIONS

A. Kholkin[1,2], S. Vasilev[2], A. Nuraeva[2], D. Vasileva[2], S. Kopyl[1], P. Zelenovskiy[2], F. Salehli[3], A. Krylov[4], S. Krylova[4] and V.Ya. Shur[2]

[1]*Dept. of Physics & CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*

[2]*Institute of Natural Sciences, Ural Federal University, 620000 Ekaterinburg, Russia*

[3]*Physical Engineering Department, Istanbul Technical University, Masta 346999 Istanbul, Turkey*

[4]*Kirensky Institute of Physics SB RAS, Krasnoyarsk 660036, Russia*

kholkin@ua.pt

Recently, short aromatic peptides have attracted significant interest because they can spontaneously form fascinating discrete and well-ordered structures at the nanoscale: nanotubes, nanospheres, nanofibrils, and hydrogels [1]. Peptide nanotubes (PNTs) based on diphenylalanine (FF) possess unique biological and physical properties such as inherent biocompatibility, high aspect ratio, remarkably rigid structure useful for many technological applications [2]. Strong piezoelectricity found recently in FF PNTs adds a new important functionality required for the development of biologically compatible sensors, actuators and micromechanical systems [3]. Piezoefect was found to be surprisingly stable as a function of temperature and applied electric field [4] being strongly anisotropic [5] and size dependent [3]. Higher chemical reactivity of PNTs as compared to carbon nanotubes (CNTs) or silicon nanowires makes it easier to carry out their modification with receptor molecules, and more versatile synthesis protocols, whereby a variety of novel biomedical devices can be produced. Recent advances in the growth process [6] have allowed studying other functional properties such as pyroelectricity and photoluminescence [7]. Multiple piezoelectric resonances were observed in PNTs thus proving there attractiveness for future generation of chemical sensors and biosensors [8]. In this presentation, apparent ferroelectric and piezoelectric properties of PNTs will be mainly discussed based on the nanoscale piezoelectric measurements, Raman spectroscopy, and dielectric relaxation focusing on the nature of the phase transitions and origin of polar state in this technologically important material.

Acknowledgement

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STRUCTURE AND TUNNELING OF METHYL GROUPS IN MOLECULAR COMPLEXES CONTAINING 2-METHYLPYRAZINE, 2,3,5-TRIMETHYLPYRAZINE AND ORGANIC ACIDS

M. Rok[1], G. Bator[1], W. Sawka-Dobrowolska[1], P. Durlak[1],
W. Medycki[2], L. Sobczyk[1] and M. Zamponi[3]

[1]*Faculty of Chemistry, University of Wroclaw, Joliot-Curie 14, 50-383 Wroclaw, Poland,*
[2]*Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznań, Poland*
[3]*Jülich GmbH, Jülich Centre for Neutron Science, outstation at FRM II, Lichtenbergstr. 1, 85747 Garching, Germany*
magdalena.rok@chem.uni.wroc.pl

Recently a great interest of researches has been focused on organic materials exhibiting semiconducting or ferroelectric properties. In investigated materials the hydrogen bonds play a crucial role. Their electrical properties seem to be a result of the proton dynamics in the strong or medium hydrogen bonds formed between the base and acid molecules. In the adducts of simple amines with organic acids, the conventional strong O–H···N or N–H···O hydrogen bonds are responsible for the infinitive chains formation. Furthermore, in a designing of the novel organic materials with the desired electrical or optical properties not only a forecast of the strength of hydrogen bonds is important but also unconventional C–H···X and aromatic π-π stacking interactions should be considered. From our view point, the methyl derivatives of pyrazine are intriguing precursor for molecular complexes, where the influence of the weak hydrogen bonds on the material properties evoke great interest [1]. The molecular complex formation in the solid state substantially changes the symmetry of the molecule. Moreover, changes in the environment of methyl groups affect their dynamics. The parameters of the methyl ($-CH_3$) group rotational potential may be a probe of both the charge transfer phenomenon and the local contacts in the crystal. In our opinion, the techniques of the inelastic neutron scattering have a particular significance in determination of the methyl group dynamics, which will be highlighted in this report.

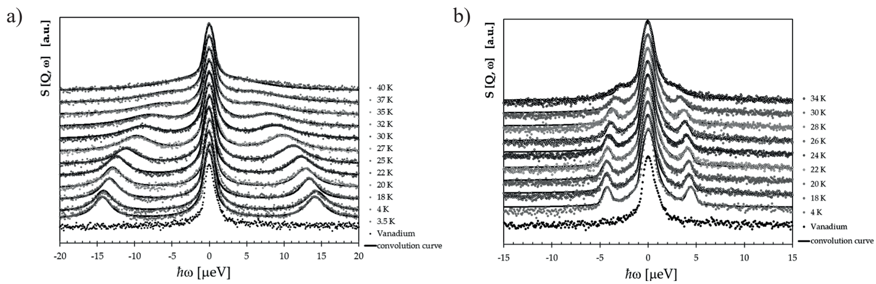

Fig. 1. Tunneling results for (a) 2MP·CLA and (b) TMP·BRA complex at several temperatures in the energy range ±20 and ±15 μeV, respectively [2].

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MULTIFERROICITY IN ORGANIC MOLECULAR-IONIC SALT

A. Piecha-Bisiorek[1], R. Jakubas[1], A. Białońska[1] and P. Zieliński[2]
[1]*Faculty of Chemistry, University of Wrocław, Joliot-Curie 14, 50-383 Wrocław, Poland*
[2]*The H. Niewodniczański Institute of Nuclear Physics, PAN, ul. Radzikowskiego 152, 31-342 Kraków, Poland*
anna.piecha@chem.uni.wroc.pl

The occurrence of ferroelectricity in the 'small-molecule' organic compounds has been known for almost a century. However, none of the previously obtained materials exhibited as good dielectric parameters, e.g. stable spontaneous polarization, as the inorganic oxide materials of the perovskite type (e.g $BaTiO_3$). Rich variety of useful physical properties of those compounds such as ferroelectricity, superconductivity, luminescence to name just a few, make them presently one of the most utilized groups of inorganic compounds.
Recent developments in the search for new, environment-friendly ferroelectrics have led to the discovery of very promising single- and two-components polar materials, which can compete successfully with the above mentioned inorganic compounds. The first of those materials, croconic acid, whose ferroelectric properties have been studied by S. Horiuchi et al., shows the highest value of spontaneous polarization among all pure organic molecules (ca. 20 $\mu C/cm^2$) [1]. Other two-component organic ferroelectrics, diisopropylammonium chloride (DIPAC) [2] and diisopropylammonium bromide (DIPAB) [3,4], belong to the group of molecular-ionic compounds and their parameters (especially for DIPAB) turned out particularly interesting. The DIPAB is characterized by an extremely high value of the spontaneous polarization (23 $\mu C/cm^2$), a high Curie temperature (426 K), a high dielectric constant, small dielectric losses and a low coercivity field.
A number of the newly synthesized materials show a symmetry-induced coupling of ferroelectricity to a macroscopic strain. The materials fall, thus, into the category of multiferroics, in the instance ferroelectric and ferroelastic. In most cases the spontaneous strain is a secondary order parameter. In this note, however, we present a new material in which the elastic degrees of freedom seem to play the essential role giving rise to a domain pattern resembling that of martensitic phase transitions, whereas the ferrolectricity appears as a side effect [5].

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POSTER - 59

EXPERIMENTAL EVIDENCE OF A TWOFOLD ORDER-DISORDER STRUCTURAL PHASE TRANSITION SEQUENCE IN PEROVSKITE-LIKE $[(CH_3)_2NH_2][Mn(HCOO)_3]$

S. Yáñez-Vilar[1,2], L.C. Gómez-Aguirre[3], B. Pato Doldán[3], M. Sánchez-Andújar[3], J. Mira[1], **J. Agostinho Moreira[2]**, A. Almeida[2] and M.A. Señarís-Rodríguez[3]

[1]*Department of Applied Physics, University of Santiago de Compostela, 15782, Santiago de Compostela, Spain*

[2]*IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia, Faculdade de Ciências da Universidade do Porto, 4169-007, Porto, Portugal*

[3]*Department of Fundamental Chemistry, University of A Coruña, 15071, A Coruña, Spain*

jamoreir@fc.up.pt

Metal-organic frameworks (MOFs) have opened up new possibilities to achieve hybrid materials with a rich variety of functional and even multifunctional properties [1]. Among them, the dense MOF, with formula $[(CH_3)_2NH_2][M(HCOO)_3]$ (with $M^{2+} = Mn^{2+}$, Fe^{2+}, Co^{2+} and Ni^{2+}), exhibits perovskite ABX_3 architecture (where $A = [(CH_3)_2NH_2]^+$, $B = M^{2+}$, $X = HCOO^-$) and interesting physical properties, combining structural flexibility, good stability, low density and cooperative magnetic and electrical properties, which may be coupled together. Among these compounds, $[(CH_3)_2NH_2][Mn(HCOO)_3]$ has been extensively studied, as this material exhibits a structural phase transition at $T_C = 185$ K, and a magnetic transition at $T_N \approx 8.5$ K [2]. The structural phase transition occurring at T_C is associated with the freezing of the rotations of the $(CH_3)_2NH_2$ molecule, placed in the A-site cavities of the $Mn(HCOO)_3$ framework. The freezing of the dimethylammonium molecule is a consequence of the establishment of hydrogen bonds between the $(CH_3)_2NH_2$ and HCOO units. This freezing process has been associated with the loss of inversion center required for the stabilization of a ferroelectric phase, though of an improper character. In this contribution, we report an experimental study of the phase sequence in $[(CH_3)_2NH_2][Mn(HCOO)_3]$ single crystals, through dielectric and Raman spectroscopies. The softening of a relaxation mode evidences the order-disorder nature of the structural phase transition at T_C. A detailed analysis of the Raman bands assigned to NH_2, COOH and CH_3 vibrations modes gives strong evidence for a twofold order-disorder structural phase sequence in this compound, associated with the establishment of hydrogen bonds at $T_C = 185$ K and $T_1 = 165$ K. Moreover, the ferroelectric nature of the low temperature phases will be discussed.

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ELECTRIC CONDUCTIVITY AND PROTON DYNAMICS IN SUPERIONIC $(NH_4)_4H_2(SeO_4)_3$

M. Zdanowska-Frączek[1], K. Hołderna-Natkaniec[2], Ł. Lindner[1] and Z. Czapla[3]

[1]*Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland*

[2]*Department of Physics, Adam Mickiewicz University, Poznań, Poland*

[3]*Department of Physics, Opole University of Technology, Opole, Poland*

mzf@ifmpan.poznan.pl

$(NH_4)_4H_2(SeO_4)_3$ (abbreviated as TAHSe) belongs to a hydrogen sulfates and selenates family crystals with general formula $M_xH_y(XO_4)_{(x+y)/2}$ (M=K, Rb, Cs, NH4, X=S, Se) which exhibit high protonic conductivity in superprotonic phase. The crystal undergoes a superionic phase transition at $T_s = 378$ K. The transition is accompanied by an increase of the conductivity by more than three orders of magnitude and above T_s the conductivity is isotropic and characterized by low activation energy of 0.27 eV. It was suggested that the phase transition is related to order or disorder of SeO_4H^{-1} or NH_4^+ ions however, these ions dynamics is still discussed. After the slow heating-cooling cycle a great thermal hysteresis of the conductivity is observed with $\Delta T_s \sim 30$ K.

Our interest of this particular system has been stimulated by recent kinetic studies performed in our laboratory. In present contribution the dynamical properties of NH_4^+ ions have been examined due to see which role, if any, they play in superionic phase transition observed in this material. We report the detailed experimental studies concerning the crystal electrical and dynamical properties. The electric conductivity measurements of the $(NH_4)_4H_2(SeO_4)_3$ crystal in high temperatures, above 260 K up to 400 K, were carried out by means of impedance spectroscopy. Independently, especially the dynamics of the NH_4^+ cations as well as the local proton motion have been studied by means of ^{1}H solid-state NMR performed in a wide range of temperatures. The results of both methods have been correlated and gave evidence that the orientational disorder of NH_4 tetrahedra is responsible for the fast proton conductivity.

On the basis of obtained results the following conclusions can be drawn: the change in the electric properties of $(NH_4)_4H_2(SeO_4)_3$ from an insulator to a superionic conductor is accompanied by changes in the anionic structure [1-3] i.e. from trimers formed by three SeO_4 tetrahedra linked with two short hydrogen bonds to dimers, which leads to reorganization of hydrogen bond network and consequently to changes in the NH_4^+ cation sublattice dynamic from the ordered to the disordered state. The process is accompanied by a chemical exchange of protons and proton diffusion within the hydrogen bond system. The NH_4^+ cations diffuse above $T_s = 378$ K in the bulk of the crystal, in superionic phase.

The form of the ^{1}H NMR signal, as well as the line width and second and fourth moment of the line was considered in the time scale at constant temperature due to yield information on the low conducting phase recovery process. The possible conduction process scenario is proposed and discussed.

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INVITED LECTURE

FERROELECTRIC DOMAIN STRUCTURING FOR PHOTONIC APPLICATIONS

K. Gallo
Department of Applied Physics, KTH – Royal Institute of Technology, 10691 Stockholm, Sweden
gallo@kth.se

Nonlinear optics has been the main driver for the convergence of ferroelectric science and optics on $LiNbO_3$ materials [1-2]. In such crystals, the nonlinear optical tensor changes sign upon reversal of the spontaneous polarization, which makes ferroelectric domain structuring a powerful tool to engineer the nonlinear optical response and realize compact and efficient photonic devices for laser frequency conversion [3], all-optical signal processing in telecom systems [4] and quantum optics [5].

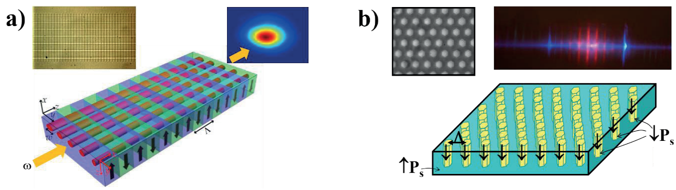

Fig. 1. a) Periodically poled $LiNbO_3$ waveguide chips for all-optical signal processing, b) hexagonally poled ferroelectric domain lattices for multiple-beam optical frequency conversion.

The presentation will discuss recent developments and current challenges to combine optical and ferroelectric functionalities on the $LiNbO_3$ technology platform, taking advantage of nanotechnology and integrated optics. In particular it shall address combining ferroelectric domain engineering with optical waveguide structures [4,6] and pushing the technology of two-dimensional poling to realize novel types of nonlinear photonic crystals [3,7].

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KEY LECTURE

CHARGED DOMAIN WALLS IN FERROELECTIRCS

T. Sluka

Ceramics Laboratory, EPFL - Swiss Federal Institute of Technology, 2015 Lausanne, Switzerland

Tomas.sluka@epfl.ch

Charged Domain Walls (CDWs) in ferroelectrics can possess metallic conductivity and can be created, displaced and erased inside a monolith of nominally insulating materials [1], therefore they are promising elements for the envisaged reconfigurable nanoelectronics [2]. Indeed, highly elevated and in some cases non-thermally activated conductivity was observed at CDWs in proper [3], improper [4] and hybrid-improper ferroelectrics [5]. The progress in understanding and towards exploitation of CDWs is hindered by the absence of practical CDW formation techniques. Here we introduce a set of methods which allow creating electronically compensated CDWs. The methods range from the use of defect ionization and migration [6], charge injection from a scanning probe tip [7], up to free-carrier generation with superbandgap illumination and the use of inhomogeneous electric fields and electron injection inside nanoscale solid structures. It will be shown that CDWs can be reliably produced in forms of large regular patters [6] and few-nanometes long precisely positioned channels [7]. These methods open the doors to the advanced investigation of CDWs and their potential technological exploitation.

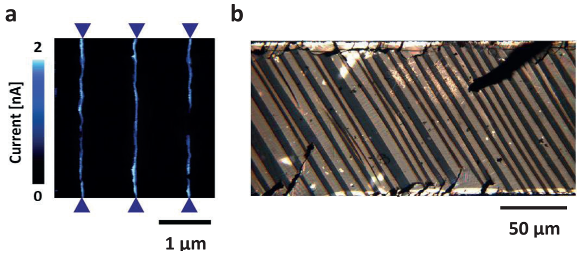

Fig. 1. (a) Conductive atomic force microscopy image of artificially created CDWs in 45 nm $(001)_c$ thick $BiFeO_3$ film on 5 nm $SrRuO_3$ electrode and $DyScO_3$ substrate [6], (b) Optical image of superbandgap illumination-created CDWs in $(111)_c$ $BaTiO_3$ single crystal.

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ULTRAVIOLET LIGHT INDUCED FORMATION OF CHARGED DOMAIN WALLS

P.S. Bednyakov[1,2], T. Sluka[2], A.K. Tagantsev[2] and N. Setter[2]
[1]*Institute of Physics of the Czech Academy of Sciences (FZU AV ČR)*
[2]*Swiss Federal Institute of Technology (EPFL)*
bednyakov@fzu.cz

Charged domain walls (CDWs) in proper ferroelectrics were shown recently to possess metallic-like conductivity [1]. Unlike conventional heterointerfaces, these walls can be displaced inside a dielectric by an electric field, which is of interest for future electronic circuitry. In addition, theory predicts that CDWs may influence the electromechanical response of ferroelectrics, with strong enhancement upon increased CDW density [2]. The progress towards CDW exploitation is, however, hindered by the complications of practical CDW engineering techniques.

Here we present a simple room-temperature bulk method which creates regular patterns of electron-hole compensated CDWs in crystals of prototypical proper ferroelectric $BaTiO_3$ (Fig.1). The procedure of CDWs preparation is based on frustrative poling across the phase transition from orthorhombic to tetragonal phase of $(111)_c$ oriented $BaTiO_3$ single-crystal. Unlike the case of electron-ion compensated CDWs described in [3], where main screening charges are electrons and mobile ionized donors, this method provides generation of free charge carriers by ultraviolet light illumination. In this case CDWs obtained with such method are compensated by electrons and holes and presumably have different properties.

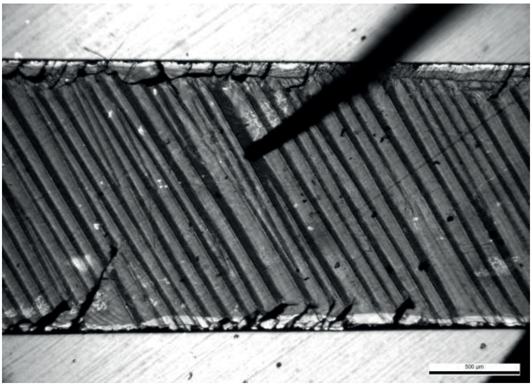

Fig. 1. Pattern of CDWs in $(111)_c$ oriented $BaTiO_3$ single-crystal obtained by frustrative poling procedure across the phase transition from orthorhombic to tetragonal phase under UV light illumination.

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ISING LINES: NATURAL TOPOLOGICAL DEFECTS WITHIN FERROELECTRIC BLOCH WALLS

V. Stepkova, P. Marton and J. Hlinka
Institute of Physics, The Czech Academy of Sciences, Na Slovance 2, 182 21 Prague 8, Czech Republic
stepkova@fzu.cz

Nowadays a great attention is paid to the investigation of domain structures and domain wall properties as well as to the formation of vortex domain states. One of the most intriguing recent result in this research field is the prediction of chiral Bloch-like domain walls in $BaTiO_3$ and $PbTiO_3$ low temperature phases based on Ginzburg-Landau-Devonshire model and first principles calculations [1-7].
The recent theoretical analysis of this new kind of domain walls for $BaTiO_3$ has predicted the possibility of chiral-to-achiral symmetry-breaking phase transitions induced by the temperature, stress or domain wall rotation and the possibility of one-dimensional topological defects appearance within the walls [5-7]. Here we use the Ginzburg-Landau-Devonshire modelling and demonstrate the possibility of interesting stable defect existence within the 180° Bloch-like domain wall in rhombohedral $BaTiO_3$, analyze its structure and properties. Some of the results related to Ising-line study have been published in [8].

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KEY LECTURE

CHARGE ORDERING AND CHARGE FLUCTUATIONS IN MOLECULAR CONDUCTORS

R. Świetlik
Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznań, Poland
swietlik@ifmpan.poznan.pl

The charge ordering (CO) in low-dimensional organic conductors, i.e. transition from uniform to non-uniform charge distribution on molecules in conducting chains or layers, attracts considerable attention since it is directly related with the pure electronic ferroelectricity, an interesting phenomenon of considerable fundamental and technological importance [1]. Temperature-induced transitions to the CO state were discovered in many charge-transfer salts formed by electron-donor tetrathiafulvalene (TTF) derivatives with different acceptors. It is generally assumed that on-site and inter-site Coulomb repulsions between charge carriers are mainly responsible for the CO effect, nevertheless donor-acceptor interactions play also an important role. Additionally, in many conductors considerable charge fluctuations are observed which usually coexist with the CO state. It was suggested that the charge fluctuations can mediate superconductivity in some salts formed by the organic donor bis(ethyleno)tetrathiafulvalene (BEDT-TTF). Both the CO and charge fluctuations have a strong influence on electronic and vibrational spectra of these salts: strong modifications of charge-transfer bands and vibrational features assigned to the C=C stretching of TTF core are seen.

At first, the CO was discovered in a series of quasi-one-dimensional (1D) salts $(TMTTF)_2X$ (TMTTF = tetramethyl-tetrathifulvalene; X= AsF_6, PF_6, SbF_6,...) and then it was shown that the effect is responsible for the electronic ferroelectricity [1]. A specific material is the 1D molecular metal $(TTM\text{-}TTF)I_3$ in which ferroelectric properties are due to an intramolecular CO [2]. Recently, we have found strong charge fluctuations in pseudo-1D organic semiconductors $(tTTF)_2X$ (X = Br, I; tTTF = trimethylene-tetrathiafulvalene) in which donors are arranged in dimeric $(tTTF)_2$ units. IR and Raman bands attributed to the C=C stretching vibrations as well as charge-transfer bands seen in IR spectra provide a clear evidence that the charge density in $(tTTF)_2$ dimers is distributed non-uniformly and undergoes strong fluctuations [3].

The CO and charge fluctuations were also discovered in many quasi-two-dimensional BEDT-TTF salts with the so-called α-, β"- and θ-type structures of conducting layers. The existence of electronic ferroelectricity was proved in α-, and θ-type salts and also in a group of κ-type BEDT-TTF salts [1]. Recently, our IR and Raman studies of the dual-layer organic metal $(tTTF\text{-}I)_2ClO_4$ have shown an unusual type of charge fluctuations, i.e. the inter-layer fluctuations. In this compound an important role is played by strong I···O halogen bond interactions between layers which strongly contribute to a small inter-layer charge-transfer interaction [4].

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STRUCTURE, ELASTICITY AND PHASE TRANSITIONS IN LIQUID CRYSTALS WITH DEFORMATIONS

A.V. Emelyanenko and N.V. Kalinin
Lomonosov Moscow State University, Moscow, Russia
emel@polly.phys.msu.ru

A molecular-statistical theory describing the liquid crystal complexes with deformations is proposed. An influence of the anisotropic properties and curvature of the surface on the nematic order parameters of liquid crystal is investigated. The order parameters and elastic constants are evaluated in the framework of a unified approach based on the features of the pair interaction potentials of individual liquid crystal molecules. We explain the two-step heat-driven transformation from the nematic phase into the isotropic phase, which is observed experimentally in [1]. It is shown that, in contrast to the case of flat surfaces [2,3], the transition from nematic phase to the isotropic phase near the strongly distorted surface (the first step) happens at lower temperatures than the transition in the bulk of liquid crystal (the second step). The molecular features responsible for the nematic order parameters change at both transitions and for the temperature range between two transitions are outlined.

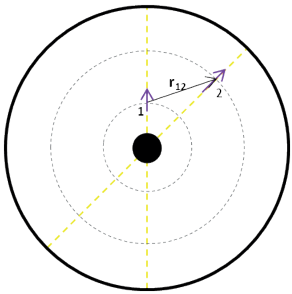

Fig. 1. Spherical nanoparticle in the centre of a large spherical nematic droplet.

A correlation between the elastic constants and the constants responsible for propagation of the order parameters from the surface to the bulk of liquid crystal is found. Both the elastic constants and the propagation constants are evaluated on the basis of the symmetry aspects of pair potentials of the individual liquid crystal molecules [4,5].

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4'-(4-ETHOXYAZOBENZENE) ALKANOATES. SYNTHESIS, MESOMORPHISM AND *trans-cis-trans* ISOMERISATIONS

E. Szypszak, I. Niezgoda and **Z. Galewski**
Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland
Zbigniew.galewski@chem.uni.wroc.pl

The liquid-crystalline compounds which were synthesized as a derivatives of azobenzene group belong to polyfunctional materials with their interesting physical properties. In this decade they are particularly intensively studied because of their many applications, especially in modern optics [1].

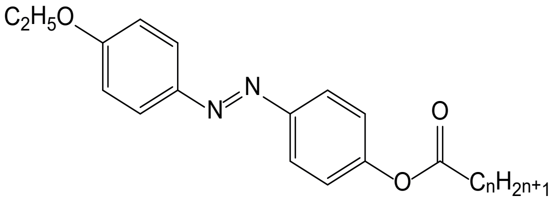

Fig. 1. Chemical structure of synthesized and investigated homologues series of azobenzene derivatives.

The main aim of this study is to investigate mesogenic properties new homologous series (19 derivatives) 4'-(4-ethoxyazobenzene) alkanoates. On the basis of three used methods (calorimetry - DSC, polarizing microscopy - POM and thermo-optical analysis - TOA) there were investigated and described parameters of phase transitions. In the investigated series only nematic mesophase was observed. This is expected result because in similar series with longer alkyloxy chain, 4 '- (4-butoxyazobenzene) alkanates, there was only a nematic phase observed, as well [2].
Derivatives of azobenzene moiety behave very interesting trans-cis-trans isomerization process. Their kinetics is characterized by two kinetics constant. Influence of the alkyl chain length on these parameters are discussed [3].

Acknowledgements
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BROADBAND DIELECTRIC SPECTROSCOPY OF $BaTiO_3$-$PbMg_{1/3}Nb_{2/3}O_3$ CERAMICS

V. Bovtun[1], J. Suchanicz[2], M. Kempa[1], D. Nuzhnyy[1], K. Konieczny[2],
T. Ostapchuk[1], J. Petzelt[1] and S. Kamba[1]
[1]*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*
[2]*Institute of Technics, Pedagogical University, Cracow, Poland*
bovtun@fzu,cz

We expand the recently published study of ceramic solid solutions of (1-x)$BaTiO_{3-x}PbMg_{1/3}Nb_{2/3}O_3$ (BT-xPMN) [1] with dielectric experiments in the high-frequency, microwave and THz ranges and present here the broadband dielectric spectra (10^1 - 10^{12} Hz) of BT-xPMN with x = 0.075, 0.10 and 0.15.
Dielectric dispersion is observed in all BT-xPMN compositions at temperatures from 100 K to 450 K in the whole investigated frequency range. In contrast to relaxor ferroelectric PMN [2], the ε'(T) maximum does not shift remarkably with increasing frequency up to 1 GHz for the x = 0.075, 0.10 compositions and only small shift is observed for the x = 0.15 one. The main dispersion takes place in the 10^9 - 10^{12} Hz range (Fig. 1), similar to that in the ferroelectric BT ceramics. THz spectra show presence of the relaxation (central) mode besides the soft phonon one, similar to that observed in the tetragonal BT [3] and PMN [2,4].
Dielectric spectra of BT-xPMN ceramics are analyzed and compared with those of BT ceramics and PMN single crystals [2]. Origin of the high-frequency dielectric dispersion is discussed in the framework of relaxor behavior, diffused phase transition and polar nanoregions concepts.

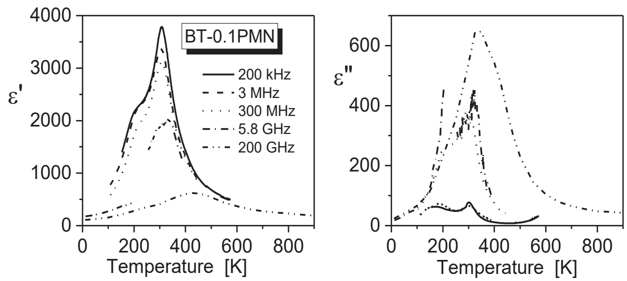

Fig. 1. Temperature dependences of dielectric permittivity and loss of BT-0.1PMN at different frequencies.

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HYPER-RAMAN SCATTERING IN QUEST FOR A_u PHONONS IN ORTHORHOMBIC $PbZrO_3$

I. Gregora[1], B. Hehlen[2], J. Hlinka[1], T. Ostapchuk[1] and E. Buixaderas[1]
[1]*Institute of Physics, Czech Acad. Sc., Prague, Czech Republic*
[2]*Laboratoire Charles Coulomb UMR5521 CNRS-UM2, Université Montpellier 2, Montpellier, France*
gregora@fzu.cz

Orthorhombic lead zirconate $PbZrO_3$ (T < ~500 K) is a very interesting anti-ferroelectric material. Its phonon spectra have been investigated in our group by IR, terahertz and Raman spectroscopy. Identification of all 117 optical phonons ($16A_g+16B_{1g}+14B_{2g}+14B_{3g}+12A_u+11B_{1u}+17B_{2u}+17B_{3u}$) is a challenging task. Most of the IR- and Raman-active species have been identified [1,2]. Our goal was to use Hyper-Raman scattering (HRS) at low temperatures to identify the remaining "silent" A_u modes, inaccessible by other spectroscopic techniques, and independently check the IR data.

Reliable observation of A_u modes is complicated by several problems: a) there is no scattering configuration allowing observation of A_u modes alone, b) identification of the B_u modes is complicated by directional dispersion, c) depolarization effects due to finite depth of the HRS focal point below the crystal surface, d) inherent polydomain structure of the samples.

A typical low-temperature HRS spectrum in crossed polarization configuration is shown in Fig. 1.

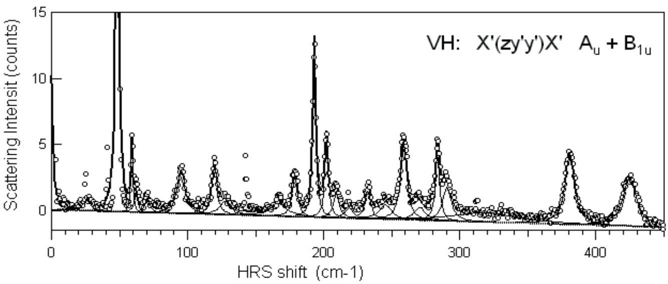

Fig. 1. Example of an HRS spectrum of $PbZrO_3$ at 20 K (directions x' and y' are rotated by 45°). All spectra were fitted by a sum of damped harmonic oscillators.

Detailed analysis of the spectra aiming at identification of "elusive" A_u, taking into account to the expected directional dispersion as calculated from the infrared data [2], will be reported.

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TEMPERATURE RAMAN SCATTERING STUDY OF BBN CERAMICS

A. Krylov[1], M. Adamczyk[2], L. Kozielski[2], A. Oreshonkov[1], A. Shabanov[1], A. Vtyurin[1] and **S. Krylova[1]**

[1]*L.V. Kirensky Institute of Physics SB RAS, s. Akademgorodok 50/38, Krasnoyarsk, 660036, Russia*

[2]*University of Silesia, Technology and Mechatronics Institute Electroceramics and Micromechatronics Division, ul. Śnieżna 2, Sosnowiec 41-200, Poland*

slanky@iph.krasn.ru

$BaBi_2Nb_2O_9$ ceramics belongs to the Aurivillius family. Aurivillius has presented mixed bismuth oxides with layer lattices in 1950 [1]. They have a very anisotropic structure consisting of oxygen octahedral blocks interleaved with $(Bi_2O_2)^{2+}$ layers. In 1961 Smolensky A. et al. have published the paper on ferroelectric properties of these materials [2]. At present the layer structured ferroelectric compounds are one of the most technologically interesting materials for non-volatile ferroelectric random access memory application [3]. Other significant factor is absence lead ions in the Aurivillius structures. Macquart R. et al. have shown the presence of a diffused crystallographic phase transition near room temperature in $BaBi_2Nb_2O_9$ [4]. Authors believe this is from the paraelectric I4/mmm structure to the ferroelectric I4mm structure. D. Nuzhnyy et al. suggested an existence of polar clusters in the paraelectric phase, whose dynamics should be in origin of the (critical) relaxations and which change into ferroelectric domains below the phase transition. For such a scenario, the usual classification into displacive and order-disorder structural transitions is no more appropriate [5].

To understand the temperature phase transition mechanisms in the $BaBi_2Nb_2O_9$ ceramics the Raman spectra were studied at temperature range from 8 to 550 K. The spectra in the 180 geometry were recorded on a Horiba Jobin Yvon T64000 spectrometer. The temperature studies were performed using an ARS CS204 X1.SS closed cycle helium cryostat. Raman spectra assignments have been performed. Detailed analysis of the line positions changes has been performed. The significant changes with temperature have been observed in the low wavenumber part of the spectrum. This part of the spectrum dues to vibrations of lattice and bismuth. The lattice vibration spectra in I4/mmm and I4mm phases were calculated. Comparative analysis of experimental and calculated spectra was made. It was shown that significant changes of spectra with temperature decreasing occur in low wavenumber range up to 200 cm^{-1}. There are lattice vibrations and vibrations of bismuth ions in this part of the spectra. Evident changes of spectra in cooling occur in the range from 500 to 700 cm^{-1}. This part of spectra is related to vibrations of oxygen ions.

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PHASE TRANSITIONS IN $PbZr_{0.72}Sn_{0.28}O_3$ SINGLE CRYSTALS STUDIED BY RAMAN SPECTROSCOPY

I. Jankowska-Sumara[1], M.-S. Jeong[2], J.-H. Ko[2] and A. Majchrowski[3]
[1]*Institute of Physics, Pedagogical University of Cracow, Kraków, Poland*
[2]*Department of Physics, Hallym University, Chuncheon, Korea*
[3]*Institute of Applied Physics, Military University of Technology, Warszawa, Poland*
ijsumara@up.krakow.pl

We have investigated single crystals of $PbZr_{0.72}Sn_{0.28}O_3$ by means of optical microscopy and micro-Raman scattering in the temperature range from 80 to 830 K. The frequencies of the Raman lines are analyzed and discussed in terms of the sequence of structural phase transitions. It was found that Raman spectrum displays important changes near 440 K, 480 K and 493 K. The incorporation of Sn^{4+} ions more than 25 mol% into the structure of $PbZrO_3$ enhances polar fluctuations above T_C as compared to the less Sn-doped crystals [1,2]. These fluctuations lead to appearance of a ferroelastic intermediate phase below T_C. It is demonstrated that the structural phase transformation in $PbZr_{0.72}Sn_{0.28}O_3$ can be considered as the result of softening of many modes, not only the ferroelectric one.

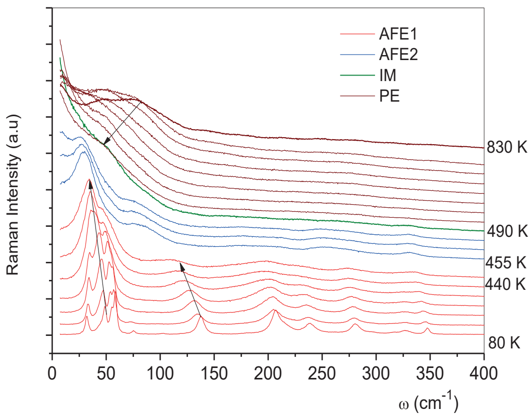

Fig. 1. The evolution of the Raman spectra for $PbZr_{0.72}Sn_{0.28}O_3$ in the A1, A2, IM and PE phases. All spectra are vertically displaced for clarity. Arrows indicate softening of certain modes.

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SPIN AND LATTICE EXCITATIONS IN THE ROOM-TEMPERATURE MAGNETOELECTRIC $(Ba_{0.2}Sr_{0.8})_3Co_2Fe_{24}O_{41}$ WITH Z-TYPE HEXAFERRITE STRUCTURE

F. Kadlec[1], C. Kadlec[1], F. Borodavka[1], J. Vít[1], Rujun Tang[2], J. Buršík[3], V. Bovtun[1], M. Kempa[1], V. Goian[1] and S. Kamba[1]

[1]*Institute of Physics, The Czech Academy of Sciences, Prague, Czech Republic*

[2]*College of Physics, Optoelectronics and Energy, Soochow University, Suzhou, China*

[3]*Institute of Inorganic Chemistry, The Czech Academy of Sciences, Řež, Czech Republic*

kadlecf@fzu.cz

$(Ba_{0.2}Sr_{0.8})_3Co_2Fe_{24}O_{41}$ crystallizes in the hexagonal Z-type hexaferrite structure and, in external magnetic fields, it counts to a rare group of room-temperature magnetoelectrics [1-3]. Below T_N = 680 K, it is a collinear ferrimagnet with spins pointing along the c axis. At T_C = 500 K, the spins reorient to a transverse conical structure and, due to the inverse Dzyaloshinskii-Moriya interaction, a ferroelectric polarization appears in a weak external magnetic field [2].

We performed measurements of ceramics samples by microwave, THz time-domain, infrared (IR), Raman and inelastic neutron scattering spectroscopies. We observed two spin excitations, whose frequencies of ca. 52 cm^{-1} and 35 cm^{-1} at 10 K decrease on heating, whereas their damping increases up to 250 K when they become smeared. The former mode is Raman active and the latter IR active only. Applying magnetic field or heating have the same marked effect on the IR-active electromagnon: the mode softens and broadens, until it disappears; if magnetic field is applied, this occurs for $H \approx 2$ T as the spin structure transforms to collinear. At still higher values of the magnetic field, a sharp ferrimagnetic resonance appears in the THz spectra. A resonance near 1 GHz, presumably of the same origin, was observed in both permittivity and permeability microwave spectra. The decrease in its resonance frequency on heating suggests that this could be a soft mode driving the spin-order phase transition at T_C.

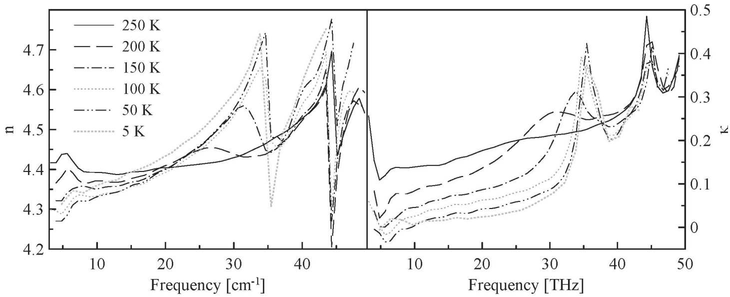

Fig. 1. THz spectra of the complex refractive index of $(Ba_{0.2}Sr_{0.8})_3Co_2Fe_{24}O_{41}$ as a function of temperature.

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POSTERS

POSTER - 1

DIELECTRIC AND SEMICONDUCTOR PROPERTIES OF $(Ba_{0.6}Pb_{0.4})TiO_3$ CERAMICS DOPED WITH GLASS IN THE RANGE OF PHASE TRANSITION

B. Wodecka-Duś, **M. Adamczyk-Habrajska** and D. Radoszewska

Institute of Technology and Mechatronics, University of Silesia, Zytnia 12, 41-200 Sosnowiec, Poland

malgorzata.adamczyk-habrajska@us.edu.pl

The aim of the poster is present the influence of the special glass, made from the mixture of simple oxides PbO-B_2O_3-Al_2O_3-WO_3, on the chemical composition, crystalline structure, microstructure, density and the electrophysical properties of the one of the members of $(1\text{-}x)BaTiO_3$-$(x)PbTiO_3$ solid solution system.

The $(Ba_{0.6}Pb_{0.4})TiO_3$ powders were obtained using the solid-phase synthesis reaction. After synthesis the initial powders were doped with the special glass, in proper stoichiometry and milled for 16 hours. Next, obtained powders were pressed in the form of disk. Prepared samples were sintered by the conventional sintering method. It was found that the ceramic material exhibited the tetragonal structure (*P4mm*) at room temperature. Variation in the concentration of special glass in the ceramic material causes a decrease in the maximum value of dielectric permittivity and shifts of the temperature of phase transition to lower value. Moreover the presence of tungsten ions leads to appearance of the PTCR effect.

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POSTER - 2

STRUCTURE AND PHYSICAL PROPERTIES OF $Ca_{1-x}Sr_xMn_7O_{12}$

S. Yáñez-Vilar[1,2], A. Nonato[3], M. Sánchez-Andújar[4], S. Castro-García[4], M.A. Señarís-Rodríguez[4], J. Mira[1], **A. Almeida**[2], J. Agostinho Moreira[2] and C.W.A. Paschoal[3]

[1]*Department of Applied Physics, University of Santiago de Compostela, 15782, Santiago de Compostela, Spain*

[2]*IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia, Faculdade de Ciências da Universidade do Porto, 4169-007, Porto, Portugal*

[3]*Departamento de Física, Universidade Federal do Maranhão, Campus do Bacanga, 65085-580, São Luis-MA, Brazil*

[4]*Department of Fundamental Chemistry, University of A Coruña, 15071, A Coruña, Spain*

amalmeid@fc.up.pt

The search for new magnetoelectric multiferroic materials, in which electric and magnetic order coexist and are strongly coupled, has attracted remarked interest due to their potential applications in magneto-electric and magneto-optical devices, "multistate" memories, etc. [1]. However, the number of multiferroic materials is small, because there are very few compounds which have both properties simultaneously and only some of them have magnetoelectric coupling.

Among them, the quadruple perovskite $CaMn_7O_{12}$, with extended formula $(CaMn_3^{3+})(Mn_3^{3+}Mn^{4+})O_{12}$, where ¾ of the A-sites are occupied by Mn^{3+} ions, ¼ by Ca^{2+} while the B sites allocate distinguishable Mn^{3+} and Mn^{4+} below 440 K. This compound shows two antiferromagnetic (AFM) helical spin ordering transitions below T_{N1} = 90 K and T_{N2} = 50 K [2]; and becomes ferroelectric at the former AFM transition, exhibiting an electric polarization of ~240 μC/cm² under a poling electric field E = 3.5 kV/cm, magnitude that is one of the highest observed so far [2-4].

In this contribution, we study the effect of the A-site strontium substitution on the physical properties of $Ca_{1-x}Sr_xMn_7O_{12}$ ($x \leq 0.3$). The ultimate goal of this research is to find out the mechanisms that drive the electric polarization in this compound.

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POSTER - 3

NEW SMART LIQUID CRYSTALLINE POLYMETHACRYLATES HIGHLY PHOTOSENSITIVE IN A BROAD SPECTRAL RANGE

A. Bubnov[1], A. Bobrovsky[2], M. Cigl[1], D. Pociecha[3], V. Hamplová[1] and V. Shibaev[2]

[1]*Institute of Physics, The Czech Academy of Sciences, Na Slovance 1999/2, 182 21 Prague 8, Czech Republic*

[2]*Faculty of Chemistry, Moscow State University, Leninskie gory, Moscow, 119992 Russia*

[3]*Laboratory of Dielectrics and Magnetics, Chemistry Department, Warsaw University, Al. Zwirki i Wigury 101, 02-089 Warsaw, Poland*

bubnov@fzu.cz

Nowadays there are enormous world-wide efforts, in both industrial and academic laboratories, to develop new so-called "smart materials'. Azobenzene-containing low-molar-mass and polymer systems present tremendous interest for the development of new materials for optics, photonics and optoelectronics. This interest is associated with fascinating photochemical properties of the azobenzene moieties, such as high quantum yield and reversibility of E-Z photo-isomerization processes, high fatigue resistance in respect of the cycles E-Z-E isomerization, pure E-Z photo-isomerization, large changes in molecular anisometry and dipole moment during E-Z isomerization. Illumination of the polarized light on amorphous or liquid crystalline (LC) films of azobenzene side chain polymers induces photo-orientation process, i.e. alignment of the azobenzene chromophores in direction perpendicular to the polarization plane of the excitation light [1]. The mechanism of this process relates to the repetitive cycles of the E-Z-E isomerization of the chromophores followed by their rotational diffusion. This effect leads to an appearance of linear dichroism and birefringence in amorphous polymer films or realignment of the chromophores in liquid crystalline films that might be used for the creation of smart materials for optical data recording and other useful applications in photonics and organic photovoltaics [2].

General objective of this work is the investigation of photo-optical properties of two novel extremely photosensitive azobenzene-containing polymers and elucidation of the effect of spacer length and LC ordering on chromophores aggregation, E-Z isomerization and photo-orientation processes in polymer films. Two photosensitive liquid crystalline (LC) azobenzene-containing polymethacrylates having different length of flexible spacer connecting chromophores with backbone spacer were synthesized and their mesophase behaviour and photo-optical properties were studied. Both polymers contain lateral methyl substituents in ortho-position of azobenzene chromophores providing high photosensitivity even in red spectral region as well as high thermal stability of photo-induced Z-form of azobenzene chromophores. It is shown, that smectic A* phase formation in films of polymer with longer spacer predetermines its quite unusual spectral response to UV and subsequent visible light actions. UV-irradiation induces not only E-Z isomerization, but also results in disruption of homeotropic alignment, whereas subsequent visible light action enables to obtain films with a low degree of chromophores orientation. The photo-orientation phenomena under the action of polarized light of different wavelength on polymer films were studied. The possibility of using red polarized light of moderate intensity for optical photo-recording on polymer films is demonstrated.

The work was supported by MEYS LH15305, RSF 14-13-00379 & CSF 16-12150S projects.

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POSTER - 4

SELF-ASSEMBLING PHOTOSENSITIVE MATERIALS AS FUNCTIONAL DOPANTS FOR ORGANIC PHOTOVOLTAIC CELLS

A. Bubnov[1], A. Iwan[2], M. Cigl[1], B. Boharewicz[2], I. Tazbir[2],
K. Wójcik[2], A. Sikora[2] and V. Hamplová[1]

[1]*Institute of Physics, The Czech Academy of Sciences, Na Slovance 1999/2, 182 21 Prague, Czech Republic*
[2]*Electrotechnical Institute, Division of Electrotechnology and Materials Science,*
M. Sklodowskiej-Curie 55/61 Street, 50-369 Wroclaw, Poland
bubnov@fzu.cz

Design of the light-harvesting and energy-converting systems belongs to one of the most highlighted fields of modern research [1-2]. Tuning and increasing the power conversion efficiency (PCE) of the organic photovoltaic (OPV) cells remains an actual and highlighted topic though several approaches has been successfully developed. Recently an effect for improving the PCE of the organic solar cells by photosensitive self- assembling materials doping has been established [3-4]. Thermal annealing within the mesophase temperature range can remove defects, optimize the morphology of the liquid crystal (LC) doped active layer of the OPV device, and hence, might be responsible for the PCE increase [3]. However, the relationship between the PCE improvement and the molecular structure of LC functional dopants is still not clear enough. The main objective of this work is to contribute to better understanding the selection rules for the specific organic molecular structures to be used as functional dopants for the improvement of the PCE of the OPV devices. Specifically the work is aimed to find a synergy between LC azo-compounds and polymer solar cells to produce smart OPV devices and to study the effect of such dopants on photovoltaic parameters.

New photosensitive LCs with a specific molecular structure have been designed in order to use them as functional dopants for the organic photovoltaic devices. As a part of basic characterisation, the self-assembling behaviour of three new organic compounds has been determined. The resulting photovoltaic devices with P3HT:PCBM active layer doped by the designed photosensitive LCs were investigated by UV-Vis spectroscopy, electrochemical measurements, cyclic voltammetry experiments, AFM surface morphology studies and impedance spectroscopy. The obtained results are summarised and discussed in terms of PCE improvement considering the specific chemical structure of the compounds used as functional dopants and the annealing temperature of an active layer. The molecular structure of compounds used as dopant has a strong effect on the value of short circuit current density. However, no significant effect of the dopant in P3HT:PCBM active layer on the open circuit voltage and fill factor has been found [5].

Authors are greatly acknowledging the financial support from the research projects: COST IC1208, MEYS LD14007, CSF 16-12150S and MEYS LH15305.

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POSTER - 5

X-RAY CHARACTERIZATION OF Co DOPED TETRAGONAL $BaTiO_3$ CERAMICS

R. Bujakiewicz-Koronska[1], L. Vasylechko[2], D.M. Nalecz[1] and A. Kalvane[3]
[1]*Institute of Physics, Pedagogical University, ul. Podchorazych 2, PL-30-084 Krakow, Poland*
[2]*Lviv Polytechnic National University,12 Bandera,79013 Lviv, Ukraine*
[3]*Institute of Solid State Physics, University of Latvia, Kengaraga 8, LV-1063 Riga, Latvia*
sfbujaki@cyf-kr.edu.pl

$BaTiO_3$:Co ceramic samples were prepared by a conventional sintering method. We present the results obtained for $BaTi_{1-x}Co_xO_3$ ($x \leq 0.1$) ceramics by the X-ray diffraction.
X-ray powder diffraction studies of $BaTiO_3$:Co specimens were performed by using Huber imaging plate Guinier camera G670 ($CuK_{\alpha1}$ radiation). Precise values of structural parameters were obtained by full profile Rietveld refinement by using WinCSD program package [1]. Silicon standard reference material SRM 640 was used as internal standard for the accurate lattice parameters determination.
The XRD patterns revealed that tetragonal $BaTiO_3$ is the main phase in all samples. However, only the less-doped $BaTi_{1-x}Co_xO_3$, x = 0.0001 specimen shows pure single-phase composition.

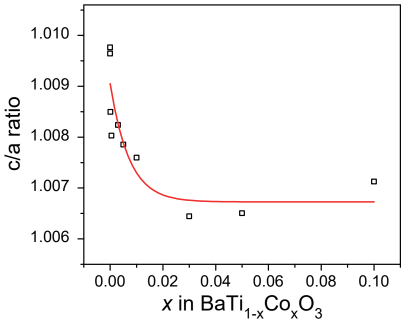

Fig. 1. Tetragonality of the $BaTiO_3$:Co_2O_3 structure as a function of nominal Co content in the $BaTiO_3$:Co_2O_3 samples.

Comparison of structural parameters of $BaTiO_3$:Co_2O_3 samples with the literature [2,3] data for the un-doped $BaTiO_3$ shows that initially the Co-doping led to decrease of the tetragonality (c/a) of the perovskite lattice. However, this effect becomes less pronounced, and practically vanishes when the nominal Co content is higher than ~ 1% (Fig. 1).

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POSTER - 6

OPTICAL QUASI-BIAXIALITY OF RELAXOR STRONTIUM-BARIUM NIOBATE SINGLE CRYSTALS

J. Dec
Institute of Materials Science, University of Silesia, PL-40-007 Katowice, Poland
jan.dec@us.edu.pl

Solid solutions of the strontium-barium niobate $Sr_xBa_{1-x}Nb_2O_6$ where $0 < x < 1$ (SBN) are environmental friendly (lead free) polar materials of oxygen octahedral family. Their potential applications are based on very attractive pyroelectric, electromechanical, electro-optic, photorefractive, and nonlinear optical and dielectric properties. Strontium-barium niobate is distinguished by its open tungsten bronze structure, i.e. the compound contains five AB_2O_6 formula units per tetragonal unit cell in which six A sites are occupied by five divalent metal atoms A. As a result the empty sites give rise to quenched electric random fields even in the stoichiometric compound. Consequently, by changing the ratio between strontium and barium components one may tune the system from ferroelectric ($x < 0.5$) to a generic relaxor ($x > 0.6$) behavior while maintaining the structure unchanged [1].

Using the Czochralski method four single crystalline compounds with nominal x = 0.40, 0.50, 0.61 and 0.75, designated hereafter as SBN40, SBN50, SBN61, and SBN75 have been grown. The crystals grown along the [001] tetragonal direction were up to 22 mm in diameter and 40 mm in length with characteristic 24 faces, free from striations and other extended defects. Density of etch pits was found to be of the order of 10^2 - 10^3 cm^{-2}.

The ferroelectric SBN single crystals are tetragonal and, according to their symmetry, are optically uniaxial. On the other hand SBN75, with typical relaxor ferroelectric properties, being tetragonal, exhibits optical features characteristic for optically biaxial systems. This kind of behavior could be considered as optical quasi-biaxiality or pseudo-biaxiality.

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POSTER - 7

PREDICTED INFRARED SPECTRA OF PZO PHONONS

Z. Dočekalová[1,2], J. Hlinka[1] and M. Pasciak[1]

[1]*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*

[2]*Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Prague, Czech Republic*

docekalova@fzu.cz

Deep and profound knowledge of phonon spectrum features can play a crucial role in discovering and understanding many properties of antiferroelectric (AFE) solids. Lead zirconate $PbZrO_3$ (PZO) usually serves as model material for studying physical phenomena concerning antiferroelectricity.

Theoretical computations within a density-functional-theory-based shell model [1] have been performed to obtain eigenenergies and eigendisplacements of each normal mode of the low-temperature phase and their properties were explored. We present the computed theoretical infrared (IR) spectra to compare the orthorhombic AFE mode structure with the cubic paraelectric (PE) one. These results were obtained using the shell-model-optimized structure and the shell-model-evaluated interatomic forces were used as an input for the PHONON program package.

Theoretical (IR) spectra were computed using both isotropic cubic and anisotropic orthorhombic Born effective charges (BEC) and were compared to the experiments [2,3]. BEC as a physical quantity is not easy to grasp and to express its physical meaning, especially for crystals with complex structure. BECs are strongly dependent on the stucture and they strongly affect the IR spectra.

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POSTER - 8

PHASE TRANSITION IN MULTIFERROIC Ni-Mn-Ga SINGLE CRYSTAL

J. Drahokoupil, P. Veřtát, K. Fabiánová and O. Heczko
Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
draho@fzu.cz

The ferromagnetic compounds derived from stoichiometric Ni_2MnGa Heusler alloy are of current interest because their large magnetoelastic response called magnetic shape memory (MSM) effect. The effect is an example of the multiferroic behaviour combining **ferro-elasticity** and **(ferro)magnetism** [1]. The alloys usually with slightly off-stoichiometric Mn-rich composition can exhibit giant (up to 12% [2]) and simultaneously fast (≈ 1 kHz [3]) straining in a moderate magnetic field (< 1 T). The effect occurs due to magnetically induced redistribution of differently oriented ferroelastic domains thanks to extremely high mobility of twin boundaries or low twinning stress. This stress can be as low as 0.05 MPa [4]. Resulting magnetic-field-induced strain (MFIS), accompanied by a reasonable force output (≈ 1 MPa) considerably exceeds the strain reachable with the best magnetostrictive and ferroelectric materials.
The martensitic phase transformation goes from high symmetry cubic phase (austenite) to low symmetry phase (martensites), e.g. with orthorhombic or monoclinic symmetry It is diffusionless, displacive, volume conserving and thermoelastic reversible within few degrees. The crystal structure of martensite determines the arrangement and complexity of twin microstructure (ferroelastic domains). As the giant field-induced strain depends on particular microstructure the detailed understanding of the crystal structure and phase transformation is crucial for the MSM effect.We focus on materials with compositions resulting in monoclinic, modulated structure so called 10M martensitic structure (see Fig. 1) at room temperature with transition temperature to austenite between 30 - 60 °C exhibiting very low twinning stress. The crystal structure, twin microstructure and phase transition will be characterized by X-ray diffraction, magnetic susceptibility, dilatometry in magnetic field and electric resistivity.

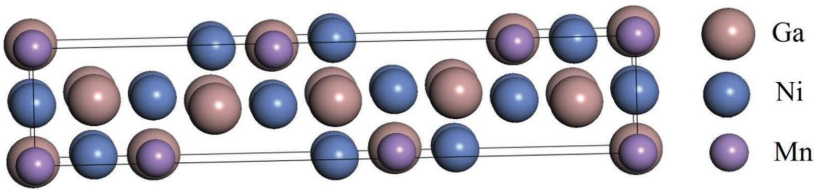

Fig. 1. The modulated 10M martensitic structure of Ni_2MnGa alloy.

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POSTER - 9

PHASE TRANSITION, THERMAL, RAMAN AND DIELECTRIC CHARACTERISTICS OF LEAD-FREE (1-x)$Na_{0.5}Bi_{0.5}TiO_3$-x$SrTiO_3$ (x=0, 0.08 and 0.1) CERAMICS

E.M. Dutkiewicz[1,2], J. Suchanicz[3], V. Bovtun[4], K. Konieczny[3], P. Czaja[3], K. Kluczewska[3], B. Handke[5], M. Antonova[6] and A. Sternberg[6]

[1]*Institute of Physics, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*

[2]*Institute of Nuclear Physics PAN, ul. Radzikowskiego 152, 31-342 Krakow, Poland*

[3]*Institute of Technics, Pedagogical University, ul Podchorazych 2, 30-084 Krakow, Poland*

[4]*Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Prague 8, Czech Republic*

[5]*Faculty of Materials Science and Ceramics, AGH-University of Science & Technology, al. Mickiewicza 30, 30-059 Krakow, Poland*

[6]*Institute of Solid State Physics, University of Latvia, LV-1063 Riga, Latvia*

erazm.dutkiewicz@ifj.edu.pl

Lead-based ceramics have been applied in several electronic devices, due to their excellent electrical properties and temperature stability [1]. However, lead-based ceramics will be tightly restricted as hazardous substances. For this reason, there is significant demand for lead-free replacement for Pb-containing materials. $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) and NBT-based materials could be good candidates for replacing compounds based on lead [2-4].
A solid-state reaction method was used to fabricate lead-free (1-x)$Na_{0.5}Bi_{0.5}TiO_3$-x$SrTiO_3$ ((1-x)NBT-xST, x=0, 0.08 and 0.1) ceramics. The XRD patterns of the obtained ceramics showed pure perovskite structure with rhombohedral symmetry at room temperature and phase transitions from rhombohedral to tetragonal and then to cubic symmetry with increasing temperature. As ST content increased, electric permittivity decreases, the maximum is broadened and shifted to lower temperature, and local anomaly shows relaxor behavior. The thermal expansion measurement results confirmed rhombohedral-tetragonal-cubic sequence phase transitions. The obtained results were discussed in term of chemical inhomogeneities, polar regions existence and strain induced by the doping.

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POSTER - 10

SUGGESTION OF THE EXTENSION OF THE DEFINITION OF A CHEMICAL REACTION

J. Fábry
Institute of Physics of the Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21 Prague 8,Czech Republic
fabry@fzu.cz

In some cases, domain reorientations which take place in ferroic crystals can be envisaged as degenerate chemical reactions though International Union of Pure and Applied Chemistry (IUPAC) [1] does not include these reorientations into this class of chemical reactions. The present contribution suggests extension of the definition of a chemical reaction: A chemical reaction is a process that results in the interconversion of chemical species or in their reorientation or in formation of an enantiomorphic structure which can take place in ferroic crystals. Examples such as hops of hydrogens that are involved in the hydrogen bonding and that take place between the donors and acceptors during ferroelastic switching are going to be discussed, e.g. H_3BO_3 [2].

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POSTER - 11

ANTIFERROMAGNETS AND FERRIMAGNETS IN HIGH MAGNETIC FIELDS

S. Fedyk[1], D.M. Nalecz[1], Z. Ropka[2] and R.J. Radwanski[1,2]
[1]*Institute of Physics, Pedagogical University, Podchorazych 2, 30-084 Krakow, Poland*
[2]*Center of Solid State Physics, S^nt Filip 5, 31-150 Krakow, Poland*
sabina.fedyk@wp.pl

We will present results of calculations of influence of high magnetic fields on antiferromagnet and ferrimagnets. We take into account the magnetocrystalline anisotropy energy, the exchange energy and the magnetostatic energy. Basically we work in the two-sublattice model in which two magnetic sublattices mutually interact. The angular dependence of the magnetocrystalline anisotropy energy is taken using Legendre'a functions. We carefully analyze the formation of a noncollinear magnetic structure under the action of the magnetic fields.
A special attention will be put for realization of physical condictions for the occurrence of the metamagnetic transition. An intention of our studies is to provide theoretical explanation of metamagnetic transitions observed in some antiferromagnets and ferrimagnets like UPd_2Al_3 and $CeRh_2Si_2$. We will try to correlate magnetocrystalline anisotropy parameters with the crystal-field parameters and low-energy electronic structure of the involved 4f /5f atom.

POSTER - 12

DIELECTRIC PROPERTIES OF POTASSIUM-SODIUM NIOBATE CERAMICS AT LOW FREQUENCIES

K. Bormanis[1], Anver I. Burkhanov[2], I. Smeltere[1], M. Antonova[1],
A. Kalvane[1] and **B. Garbarz-Glos[3]**
[1]*Institute of Solid State Physics, University of Latvia*
[2]*Volgograd State Architectural and Engineering University, Volgograd, Russia*
[3]*Institute of Engineering, Pedagogical University, Cracow, Poland*
barbaraglos@gmail.com

Studies of electrical properties of ferroelectric potassium-sodium niobate ceramics of $(K_{0.5}Na_{0.5})(Nb_{1-x}Sb_x)O_3$ (KNN-x) at x = 0.05 (KNN-5) synthesised by conventional solid state reactions with admixture of 0.5 mol% MnO_3 subjected to extended exposure to constant temperature, electric field and radiation are reported. The infra-low frequency dielectric response is studied by Sawyer-Tower techniques used to record polarisation loops under sinusoidal field of constant amplitude E of different duration. Behaviour of polarisation loops after different numbers of cycles of the sinusoidal electric field E is presented. A considerable rise of the dispersion of dielectric permittivity is observed at increasing E after the samples are held at constant temperature and constant bias field. The growth of the effective dielectric permittivity is well described by power function $\varepsilon'_{eff} = \varepsilon'_{st} + Bt^c$ (solid line) where ε'_{st} is the initial value (first cycle) of ε'_{eff}, B - experimental constant, and exponent c equal to 0.20 - 0.25 is found from analysis of approximations (the features of $\varepsilon'_{eff}(t)$ at strong and weak field intensities are the same). Restoration (growth) of polarisation by extending the time (number of infra-low frequency AC field cycles) under applied field below coercive E_c in aged materials follows the power law similar to growth at increasing the amplitude of the applied field.

POSTER - 13

FRUSTRATED SMECTIC LIQUID CRYSTALLINE PHASES IN LACTIC ACID DERIVATIVES

M. Glogarová and V. Novotná
Institute of Physics, Academy of Sciences of the Czech Republic, Prague 8, Czech Republic
glogarova@fzu.cz

In chiral liquid crystalline compounds tendencies to form helical or twisted structures and to form layers can be in contradiction. To escape from the frustration in the molecular packing the phases with regular array of defects are formed, composed of blocks of a homogeneous structure separated by twist grain boundaries (TGB).

We have prepared and studied series of compounds with the molecular core containing at least one biphenyl laterally substituted with chlorine and at least two chiral centers, one or two being the lactate group. They provide a variety of frustrated twist grain boundary (TGB) phases and quite unique phase sequences [1,2]. Some of them exhibit extremely wide TGBA phase more than 60 K broad, thus exceeding many times the widths of this phase ever found. Besides, the TGBA-TGBC-SmC*-SmC$_A$* phase sequence has not been reported for any other compound so far.

Another one-lactate-compound laterally substituted with bromine exhibits quite unique phase sequence with the re-entrant TGBA phase below the SmA phase. This phenomenon cannot be explained by interdigitation of molecules within the smectic layers that usually accompany the re-entrancy phenomena in liquid crystals known so far, because the smectic layer spacing remains equal in all phases [3].

Additionally, we have induced frustrated phases in binary mixtures of molecules with different molecular shape and chirality (non-chiral hockey-stick and chiral rod-like compound). On contrary to both components, which exhibit regular standard phases, the TGBA, TGBC and frustrated blue phases (BP) were observed in the phase diagram. Due to combination of component properties the phase sequence containing both cholesteric and antiferoelectric phase has been found in the studied binary system. Such a phase sequence cannot exist in single component liquid crystals [4].

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POSTER - 14

MECHANICAL PROPERTIES AND SUPERCONDUCTING NANOSTRUCTURES OF Cu-Ag AND Cu-Nb THIN WIRES

Z. Rdzawski[1], **W. Głuchowski**[1], W. Kempiński[2], B. Andrzejewski[2] and J. Stobrawa[1]
[1]*Institute of Non Ferrous Metals, Gliwice, Poland*
[2]*Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland*
wojciech.gluchowski@imn.gliwice.pl

Recent advances in nanofabrication of normal metal and superconducting nanostructures provided excellent test systems for practical applications and also gave unique opportunity for understanding of physical phenomena appearing in metals in confined geometries. For contemporary applications, there is a constant quest for materials of specific and very often contradictory sets of properties like high electrical and thermal conductivities combined with very high mechanical strength. On the other hand normal conducting and superconducting nanocomposites with 0-3 or 1-3 connectivity make it possible studying of charge carrier behavior in highly confined geometries. Interesting examples are one dimensional superconducting nanowires with diameters comparable to the superconducting coherence length immersed in normal conducting matrices (i.e. 1-3 connectivity) that can exhibit unique properties like, thermal and quantum phase slips, an “antiproximity effect”, “row” vortex lattices, minigap state, resistance fluctuations, shape-dependent superconducting resonances and many others.
In this work we report on manufacturing and properties of Cu-Ag or Cu-Nb composite and Cu-Nb multifilament nanowires obtained by means of innovative extrusion and compacting methods [1]. The nanostructure of Cu-Nb (Cu-Ag) fine wires was irregular with Nb (Ag) particles of globular shape and narrow filaments of the niobium or silver-rich phase (Fig. 1b). The wires derived from Cu-Nb alloys exhibited advantageous mechanical properties and relatively high electrical conductivity. Multifilament nanowires had more than 820,000 niobium nanofilaments of a diameter between 100 and 200 nm and hexagonally distributed in a pure copper matrix (Fig. 1b). These superconducting composites exhibited enhanced critical currents, critical temperature comparable to bulk Nb and microwave absorption due to vortex lattice motion or phase slips at Nb-Cu-Nb Josephson junctions.

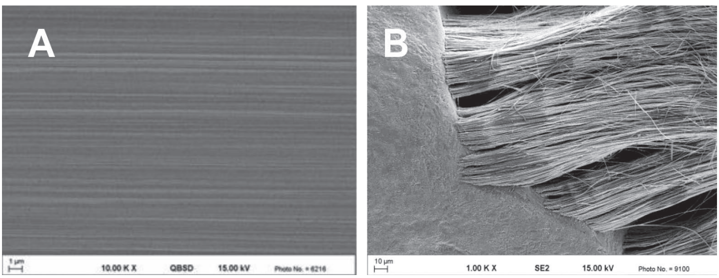

Fig. 1. Microstructure of Cu-Ag wire (a) and Nb multifilament nanowire with partially etched Cu matrix (b).

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POSTER - 15

STRUCTURE AND MAGNETIC PROPERTIES OF Nd AND Al CODOPED $SrFe_{12}O_{19}$

A. Hilczer[1], K. Pasińska[2], A. Pietraszko[2] and B. Andrzejewski[1]
[1]*Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland*
[2]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland*
ahilczer@ifmpan.poznan.pl

$Sr_{1-y}Nd_yFe_{12-x}Al_xO_{19}$ single-phase solid solution with $y \leq 0.1$ and $x \leq 2$ have been recently obtained by auto-combustion method [1,2]. Nd^{3+} doping of $SrFe_{12}O_{19}$ hexaferrite was reported to improve the coercivity, whereas nonmagnetic Al^{3+}, substituting the Fe^{3+} ions, resulted in a decrease in saturation magnetization [3]. As the magnetic properties are strongly dependent on the processing conditions we decided to apply other method and to obtain $Sr_{0.95}Nd_{0.05}Fe_{12-x}Al_xO_{19}$ solid solution by hydrothermal synthesis from precursors: $Fe(NO_3)_3 \cdot 9H_2O$ (ChemPur S.A.), $Sr(NO_3)_2$ (ChemPur S.A.), Nd_2O_3 (Alfa Aesar) HNO_3 (ChemPur S.A.), $Al(NO_3)_3 \cdot 9H_2O$ (ChemPur S.A.) and NaOH (ChemPur S.A.) with $[Fe^{3+}/Sr^{2+}] = 4$ and $[OH\text{-}/NO^{3-}] = 5$ molar ratios. The obtained solutions with x = 0.36, 0.60, 0.84 and 1.08 were characterized by X-ray diffraction (X'Pert PANalytical, CuK_α, Bragg-Brentano geometry) and scanning electron microscopy (FEI NovaNanoSEM 230). Single phase solid solution has been confirmed for all samples and the powder consisted of flower-like agglomerates composed of ~20 nm thin platelets of hexagonal shape (Fig. 1a). Physical Property Measurement System (PPMS, Quantum Design) was used for measuring magnetic properties in the temperature range from 4 to 300 K. Al-doping of $Sr_{0.95}Nd_{0.05}Fe_{12}O_{19}$ solid solution was found to modify slightly the magnetization (Fig. 1b) but the temperature variation of magnetization in FC and ZFC experiments were changed considerably.

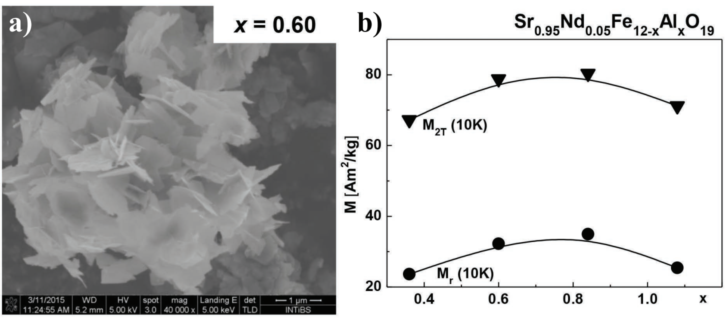

Fig. 1a SEM image of an agglomerate of $Sr_{0.95}Nd_{0.05}Fe_{11.4}Al_{0.6}O_{19}$ crystallites; 1b remanence M_r and magnetization M measured in field of 2 T at 10 K.

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POSTER - 16

BROAD-BAND DIELECTRIC RESPONSE OF $0.5Ba(Ti_{0.8}Zr_{0.2})O_3$-$0.5(Ba_{0.7}Ca_{0.3})TiO_3$ CERAMICS: SOFT AND CENTRAL MODE BEHAVIOR

S. Kamba[1], E. Simon[1], V. Skoromets[1], J. Pokorný[1], V. Bovtun[1], M. Kempa[1],
M. Savinov[1], J. Koruza[2,3] and B. Malič[2]

[1]*Institute of Physic, Czech Academy of Sciences, Prague, Czech Republic*
[2]*Institute Jozef Stefan, Ljubljana, Slovenia*
[3]*Technische Universität Darmstadt, Alarich-Weiss-Str. 2, Darmstadt, Germany*
kamba@fzu.cz

The lead-free ceramic system $Ba(Ti_{0.8}Zr_{0.2})O_3$-$(Ba_{0.7}Ca_{0.3})TiO_3$ (BZT-BCT) has a high application potential due to its exceptionally high piezoelectric coefficient d_{33} ~ 620 pC/N [1]. We have prepared ceramic samples with the chemical composition 0.5BCT-0.5BZT which corresponds to the system with the highest attainable d_{33}. The dielectric properties were probed in the frequency range from 10 Hz to 100 THz at temperatures between 10 and 900 K. We systematically investigated its lattice dynamics near structural phase transitions using THz, IR and Raman spectroscopies.

According to W. Liu et al. [1], 0.5BCT-0.5BZT ceramics undergoes two structural phase transitions from the cubic phase to the tetragonal one and then to the rhombohedral phase. Our dielectric data, however, indicate an additional low-temperature phase transition. Therefore, we propose a phase transition sequence similar to that observed in $BaTiO_3$ single crystals, i.e. from cubic to tetragonal, orthorhombic and finally to a rhombohedral phase.

Polar soft mode, which can be seen in IR and THz spectra, exhibits anomalous behavior near ferroelectric phase transitions. Nevertheless, the dielectric anomalies observed in the vicinity of all the three phase transitions are caused mainly by a dielectric relaxation (central mode) in the microwave and THz regions below the soft mode. Consequently, the phase transitions strongly resemble a crossover between the displacive and order-disorder type. The central mode appears in the THz spectra below 500 K and again disappears below 200 K. Raman spectra reveal new phonons below the cubic-to-tetragonal ferroelectric phase transition at T_C = 360 K. Some phonons shift in frequency on cooling below the orthorhombic-to-rhombohedral phase transition. The dielectric relaxation in the microwave range anomalously broadens on cooling below T_C resulting in a near-constant dielectric loss below 200 K. A similar behavior is frequently observed in ferroelectric relaxors, where the dynamics of polar clusters is responsible for such a behavior. In the ferroelectric 0.5BCT-0.5BZT, the near-constant dielectric loss comes from a broad frequency distribution of ferroelectric domain wall vibrations.

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POSTER - 17

EFFECTS OF $PbTiO_3$ DOPING ON ELECTRIC PROPERTIES OF $Na_{0.5}Bi_{0.5}TiO_3$ CERAMICS

M. Karpierz[1], J. Suchanicz[2], K. Konieczny[2], W. Smiga[2] and P. Czaja[2]
[1]*Institute of Physics, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*
[2]*Institute of Technology, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*
mkarpierz@outlook.com

Materials which have relaxor ferroelectric behavior are very attracted due to possibility of their use to production of transducers, actuators or other electromechanical devices. On the other hand, such properties occur more often in lead - based ceramics. Lead titanate-zirconate (PZT) ceramics are one of the most used ferroelectric materials [1]. The downside this ceramics is toxicity of lead and its high vapour pressure during processing. Low-lead and lead-free ceramics can be used instead of lead-based materials if their properties will be promising [2]. $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) has lately received significant attention as a prospective replacement for the universally used lead-based piezoelectric materials.
Good quality ceramics of $(1-x)Na_{0.5}Bi_{0.5}TiO_3-xPbTiO_3$ (x = 0, 0.03 and 0.05) were prepared by a conventional solid phase sintering process. The temperature dependence of dc, ac conductivity (σ_{dc}, σ_{ac} respectively), the Seebeck coefficient (α) and the value of charge carriers concentration n of these ceramics were investigated. The measurements were made in the temperature range from 30 °C to 600 °C. Dc conductivity for pure NBT possesses three linear parts with three different activation energies E_a, For 0.97NBT-0.03PT and 0.95NBT-0.05PT ceramics dc conductivity has also three linear part (three different E_a). On the other hand, ac conductivity possesses three linear part (three different E_a) for pure NBT and four (four different E_a) for other compositions. The possible origin of the observed effects was discussed. We suggest that the presented materials can be a good starting point for the development of low-lead electronic ceramics.

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POSTER - 18

DIELECTRIC PROPERTIES OF STRATIFIED POLYDOMAIN $BiFeO_3$

I. Rychetsky, **A. Klíč** and J. Hlinka
Institute of Physics, ASCR, Czech Republic
klic@fzu.cz

Effective properties (dielectric, magnetic, mechanical) of inhomogeneous materials are important for applications and so it is very desirable being able to determine them from given known microstructural parameters and from the bulk properties of homogeneous components. The inhomogeneity can be realized in many ways for example by random arrangements of anisotropic grains of polycrystal material or ceramics, or, as it is in our case, by the polydomain structure of a single crystal.
In this contribution we provide analysis of the polydomain crystal of $BiFeO_3$ in the ferroelectric rhombohedral phase *R3c*. There are 8 possible domain states with different orientation of the spontaneous polarization. Two stratified structures composed of 2 domains are studied: in the first structure the domains are separated with the equidistant uncharged 109°-DW's (Fig. 1), and in the second case with the electrically neutral 71°-DW's. The domain states are characterized with the uniaxial permittivity tensor, the stiffness tensor and nonzero piezoelectric tensor. Taking into account conditions of mechanical and electrical equilibrium the effective permittivity tensors of the both quasi-onedimensional structures were first solved analytically, and then numerically using experimental values of the material constants. It is also shown that in the limit of zero piezoelectric tensor the formulas transform to the serial and parallel capacities [1].

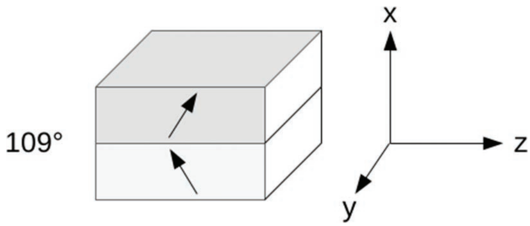

Fig. 1. 109°-DW structure.

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POSTER - 19

ELECTRICAL AND THERMAL PROPERTIES OF $Na_{1-x}Li_xNbO_3$ (x = 0.08, 0.1, AND 0.2) CERAMICS NEAR THE MORPHOTROPIC PHASE BOUNDARY

K. Konieczny and P. Czaja
Institute of Technics, Pedagogical University, ul. Podchorążych 2, 30-084 Kraków, Poland
kkoniec@up.krakow.pl

The ferroelectric with perovskite structure are very interesting materials because their strong anomalies in their physical properties, such as dielectric, electric-optical, piezoelectric, pyroelectric properties. Sodium niobate $NaNbO_3$ exhibits large number of successive phase transitions (at about: -110, 140, 190, 360, 480, 520, 575 and 641°C) and have both ferroelectric (in low temperature range) and paraelectric (up to about 480 °C) properties [1]. Lithium niobate $LiNbO_3$ is the ferroelectric with ilmenite structure. Undergoes a second order phase transition from the ferroelectric phase to paraelectric phase. The Curie temperature is about 1200°C [2]. Solid solution based on sodium niobate and lithium niobate has ferroelectric and piezoelectric properties. $Na_{1-x}Li_xNbO_3$ ceramics with composition for x = 0.08, 0.1 and 0.2 were prepared by solid - state reaction method and sintered in the temperature about 1200 °C. Structural properties, thermal properties, measurements of temperature changes of dielectric permittivity of $Na_{1-x}Li_xNbO_3$ (x = 0.08, 0.1 and 0.2) ceramics near the morphotropic phase boundary are presented. The measurements were carried out in temperature range from room temperature to 600 °C and frequency range from 0.1 kHz to 2 MHz. Modification of content ions of lithium make significant changes of electrical properties. These solid solutions show interesting properties from the point of view of the application.

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POSTER - 20

DOUBLE HYSTERESIS LOOP IN $BaTiO_3$-BASED FERROELECTRIC CERAMICS PREPARED BY HIGH ENERGY MILLING

L. Kozielski[1], I. Szafraniak-Wiza[2], T. Sebastian[3] and F. Clemens[3]
[1]Department of Materials Science, University of Silesia, 41-200 Sosnowiec, Żytnia 12, Poland
[2]Institute of Materials Science and Engineering, Poznan University of Technology, Jana Pawla II 24, 61-138 Poznań, Poland
[3]EMPA, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for High Performance Ceramics, 8600 Duebendorf, Switzerland
lucjan.kozielski@us.edu.pl

The challenge from an industrial manufacturing perspective is to shift high temperature solid state sintering to low temperature. has just become such productive and cost-effective technology to be utilized in many applications. The main advantage of this method is the room temperature process that is the most important factor in piezoelectric polymer composites technology. The second benefit is the economical usage of simple oxides in synthesis process.
In present work, the mechanosynthesis was implemented to synthesize piezoelectric powders in ceramics material technology, based on time dependant potential energy - induced solid state synthesis, was in $Ba_{0.8}Ca_{0.2}TiO_3$ and $BaTiO_3$ as for reference sample substantiated. Consequently the both lead-free materials piezoelectric material was synthesized by high-energy milling from barium, calcium and titanium oxides. However, directly after mechanosynthesis the obtained powders exhibited the perovskite structure and ferroelectric properties but unfortunately too long time milling processing induced many structural defects visible in distorted hysteresis loops.

POSTER - 21

THE INFLUENCE OF THE DYE CONCENTRATION ON THE LIQUID CRYSTALS' ORDER PARAMETER <P_2>

N. Bielejewska[1], W. Krym[2], E. Chrzumnicka[2] and **W. Kuczyński[1]**

[1]*Institute of Molecular Physics Polish Academy of Sciences, Poznań, Poland*

[2]*Poznań University of Technology, Poznań, Poland*

natalia.bielejewska@ifmpan.poznan.pl

In this work the influence of the dye additive on the liquid crystals' order parameter $\langle P_2 \rangle$ has been investigated. The knowledge of liquid crystal order parameters are crucial for their use in optoelectronics [1,2]. In present study we use different techniques, based on the measurements of the optical birefringence, absorption and emission of the polarized light, for determination of the order parameter $\langle P_2 \rangle$ as a function of temperature [3,4]. The birefringence studies were conducted with use of the plan-convex lens, Berek's compensator and photoelastic modulator (PEM). Although in measurements based on the birefringence phenomena the addition of the dye is not required, in order to be able to compare obtained results with those of the optical spectroscopy methods, the dye molecules were used as guest in guest-host mixtures of the dye and liquid crystal. In the studies the liquid crystal 4-trans-4'-n-hexylcyclohexyl-isothiocyanatobenzene (6CHBT) and two dyes: 4-dimethylamine-4'-nitrostilbene (DANS) [4] and N,N'-bis(2,5-di-tert-buthylphenyl) -3,4,9,10-perylenedicarboximide (BTBP) were used [5]. The measurements were conducted as a function of temperature for the whole region of nematic phase occurrence.

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POSTER - 22

STRUCTURAL, ELECTRIC AND MÖSSBAUER STUDIES OF 5% Fe – DOPED $BiMnO_3$

A. Leonarska[1], M. Kądziołka-Gaweł[1], A. Szeremeta[1], R. Bujakiewicz-Korońska[2], A. Kalvane[3] and A. Molak[1]

[1]*Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland*

[2]*Institute of Physics, Pedagogical University, Podchorążych 2, 30-084 Kraków, Poland*

[3]*Institute of Solid State Physics, University of Latvia, 8 Kengaraga, LV-1063, Riga, Latvia*

agnieszka.leonarska@us.edu.pl

The $BiMnO_3$-Fe ceramics were sintered at 1130 K for 6 h in ambient air. The X-ray pattern analysis shows that the ceramics consists, at room temperature, of two centro-symmetric phases. The lattice parameters are: a = 10.201(9) Å for cubic *I23* and a = 7.539(4) Å, b = 8.545(9) Å, c = 5.761(9) Å for orthorhombic *Pbam* phase [1,2]. The electric impedance was measured for f = 20 Hz - 1 MHz in the 100 - 690 K range. It was analysed with use of electric modulus formalism M"(T). The $BiMnO_3$-Fe ceramics shows two electric conductivity relaxations. One process is related to activation energy $E_{a,1}$ = 0.14 - 0.20 eV and characteristic time values $\tau_{01} = 10^{-10} - 10^{-12}$ s in 100 - 200 K range. It is deduced that Fe doping affected this relaxation process, i.e. $E_{a,1}$ value decreased and τ_{01} increased. Next process occurred in 170 - 220 K range and it exhibited $\tau_{02} = 10^{-11}$ s and $E_{a,2}$ = 0.27 eV [2]. The dc resistivity $\rho_{dc}(T)$ temperature dependence shows semiconductor features and the value $E_{a,dc}$ = 0.28 - 0.37 eV. The VRH polaron model was discussed for $\rho_{dc}(T)$ and also for the relaxations. The ^{57}Fe Mössbauer spectrum was recorded at room temperature. The spectrum shows pure electronic quadrupolar interactions. The quadrupole splitting corresponds to the asymmetrical part of the electronic hyperfine interaction between the Fe nucleus and its surrounding charges. The doublets represent iron Fe^{3+} ions distributed in the two sites, i.e. octahedral (O) and square pyramidal (P), with a preferential occupation of the P sites [3]. Moreover, a third doublet is visible in the Mössbauer spectrum. It results probably from a small admixture of another crystal phase with iron Fe^{3+} in tetrahedral coordination.

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POSTER - 23

DIELECTRIC AND FERROELECTRIC PROPERTIES OF NBT-BT SYSTEMS

U. Lewczuk[1], J. Suchanicz[2] and M. Karpierz[1]

[1]*Institute of Physics, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*

[2]*Institute of Technology, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*

urszula.lewczuk@gmail.com

Lead-based ceramics have been extensively used in electronic devices, due to their supreme electrical properties. On the other hand, lead-containing ceramics have a harmful effect on the environment, so they are not desirable nowadays. The $Na_{0.5}Bi_{0.5}TiO_3$-$xBaTiO_3$ ceramics (x=0.1, 0.135 and 0.17) were fabricated by a conventional solid phase sintering process. The dielectric and ferroelectric measurements of these ceramics were performed. The bulk density of the obtained samples exceeds 95% of the theoretical density. The ferroelectric measurements show that above the depolarization temperature, the shape of hysteresis loops is approaching that of linear dielectrics. The dielectric study correlates with the hysteresis loops measurements. The relaxor behavior of the investigated materials was revealed.

POSTER - 24

DIELECTRIC AND MAGNETIC PROPERTIES OF $BiFeO_3$-PVDF NANOCOMPOSITES

E. Markiewicz, K. Chybczyńska, B. Hilczer, M. Połomska and B. Andrzejewski
Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
ewamar@ifmpan.poznan.pl

Polymer-based nanocomposites of multiferroic $BiFeO_3$ (BFO) are considered for wide range of applications since they can be produced in form of flexible thin films. Properties of BFO composites with several non-polar polymers have been reported and only 3 papers are dealing with BFO-PVDF composites [1-3]. We studied the dielectric and magnetic response of poly(vinylidene fluoride) (PVDF) loaded with BFO crystallites with median thickness of 61 nm produced by microwave assisted hydrothermal method [4]. BFO was controlled by XRD (pure BFO), SEM (thickness distribution of the crystallites), whereas the semicrystalline PVDF was characterized by NIR Raman spectroscopy (conformations) and DSC. Radially oriented BFO/PVDF composites with (0-3) connectivity and BFO volumetric content Φ were produced by hot pressing (500 K, 600 MPa, 30 min) and covered with gold electrodes for dielectric measurements (Novocontrol GmbH, 125 K ≤ T ≤ 525 K on heating at dT/dt = 1 K/min, 0.01 Hz ≤ f ≤ 10 MHz). The dielectric response of composites was found to be determined by the response of the polymer matrix and BFO loading results in an increase in ε' and ε" values. The ε'(Φ) dependence at room temperature can be described by the logarithmic mixing rule. BFO was found also to affect the dynamics of segmental motion in the amorphous phase of the matrix: the freezing temperatures of dipolar motions are shifted upwards and the activation energy decreases with the increase in the volumetric fraction of BFO.
Magnetic properties of the composites were studied in the temperature range from 10 to 300 K with a Vibrating Sample Magnetometer probe installed on a PPMS system fitted with superconducting 9 T magnet. Ferromagnetic hysteresis loops with magnetization increasing with the BFO volumetric fraction Φ in the composites were observed and related to a surface spin disorder and incomplete spin rotation along the wave vector direction in BFO nanocrystallites.

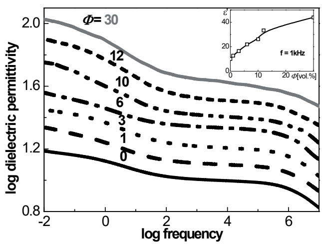

Fig. 1. logε' *versus* logf for BFO-PVDF nanocomposites of various volumetric fraction Φ at room temperature.

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POSTER - 25

FERROELECTRIC NANOCOMPOSITES ON BASE OF MAGNETIC POROUS GLASSES

E. Koroleva[1,2], **A. Naberezhnov[1,2]**, V. Nizhankovskii[3], P. Vanina[2], A. Sysoeva[1] and I. Glavatskyy[4]
[1]*Ioffe Institute, St.-Petersburg, Russia*
[2]*Peter the Great Saint-Petersburg Polytechnic University, St.-Petersburg, Russia*
[3]*International Laboratory of High Magnetic Fields and Low Temperatures, Wroclaw, Poland*
[4]*Helmholtz-Zentrum Berlin, Hahn-Meitner platz 1, D-14109, Berlin, Germany*
alex.nabereznov@mail.ioffe.ru

We have prepared a new-generation nanocomposite materials (NCM) based on magnetic micro (MIP)- and macroporous (MAP) alkali borosilicate glasses in which magnetic atoms are incorporated directly into the matrix skeleton. In these matrices, pores form a through three-dimensional dendrite system with a total porosity reaching up to 40 - 50% of the sample volume. Dielectric and magnetic characteristics of these matrices were studied, and it was confirmed that matrices demonstrate magnetic properties. The field dependences of the linear and volume magnetostriction were determined [1], that opened the way to the creation of a new class of multifunctional materials with spatially separated ferroelectric (embedded inti the pores) and magnetic (in the matrix skeleton) ordering. The presence of magnetostriction and a developed interface between embedded ferroelectrics and magnetic matrix ensure the interaction between these subsystems. In order to check for the possibility of magnetic control over the ferroelectric subsystem, nanocomposite materials have been prepared on base of macroporous magnetic glasses (Fe20MAP) with an average pore diameter of 50(5) nm, which contained embedded KH_2PO_4 (KDP) and $NaNO_2$. The dielectric response of NCM Fe20MAP+KDP have been studied in magnetic fields 0 - 12 T, the temperature dependence of order parameter in NCM Fe20MIP+$NaNO_2$ have been studied in magnetic fields 0 - 2 T by neutron diffraction.

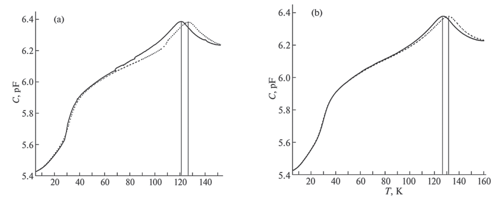

Fig. 1. Temperature dependences of capacitance C measured for Fe20MAP + KDP nanocomposite on cooling (dotted line) and heating (solid line) in (a) zero field and (b) external field of B = 10 T. Vertical lines indicate the positions of maximum on the C(T) curves.

Principle results: 1. In NCM Fe20MAP+KDP TC increases on 6 K at magnetic field 10 T. 2. Application of magnetic field 2 T to NCM Fe20MIP+$NaNO_2$ changes the dependency η(T) near the ferroelectric phase transition and decreases T_C, but at RT we have not observed any alteration of intensities of elastic peaks depending on ferroelectric order parameter.

This contribution is supported by RFBR (grant 15-02-01413)

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POSTER - 26

THE CRYSTAL FIELD EFFECTS IN HEXAGONAL 4H-$SrMnO_3$

D.M. Nalecz[1], R.J. Radwanski[1,2] and Z. Ropka[2]
[1]*Institute of Physics, Pedagogical University, ul. Podchorazych 2, PL-30-084 Krakow, Poland*
[2]*Center of Solid State Physics, S^{nt} Filip 5, PL-31-150 Krakow, Poland*
sfnalecz@cyf-kr.edu.pl

We have analyzed properties of the hexagonal 4H-$SrMnO_3$ starting by calculating the low-energy electronic structure of the Mn^{4+} ion in distorted octahedral oxygen surroundings. Similar investigation for the cubic phase C-$SrMnO_3$ we have presented in [1]. We treat the Mn^{4+} ion as the strongly-correlated $3d^3$ system with the ground atomic term 4F. 4H-$SrMnO_3$ becomes antiferromagnetic below T_N of 286 K [2]. The ^4F term is 28-fold degenerated. This degeneracy is lifted by the combined action of the dominant octahedral crystal field and off-octahedral distortions [Fig. 1].

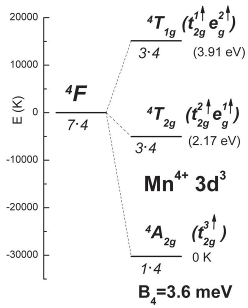

Fig. 1. The splitting of the lowest 4F electronic term of the Mn^{4+} ($3d^3$) ion in $SrMnO_3$ by the crystal-field interactions of the octahedral symmetry.

This study is concentrated on the explanation of the temperature dependence of the specific heat showing a pronounced λ-type peak at T_N [3]. We have calculated the d-electron contribution, using the crystal-field approximation [4], to the specific heat both in the antiferromagnetic and the paramagnetic states of the hexagonal polymorph 4H-$SrMnO_3$. We found that the trigonal distortion modifies the electronic structure associated with the $^4A_{2g}$ subterm largely influencing the magnetic-moment value and stabilizing direction of the magnetic moment within the elementary cell.

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POSTER - 27

SYNTHESIS AND STRUCTURE STUDIES OF $Ni_xCo_{3-x}O_4$

D. Nicheva[1,2], B. Abrashev[1], P. Ławniczak[3], Ł. Lindner[3], M. Zdanowska-Frączek[3], P. Petkov[2] and T. Petkova[1]

[1]*Institute of Electrochemistry and Energy Systems, BAS, Acad. G.Bonchev bl.10, 1113 Sofia, Bulgaria*

[2]*University of Chemical Technology and Metallurgy, 8, St. Kliment Okhridski Blvd., 1756 Sofia, Bulgaria*

[3]*Institute of Molecular Physics, PAS, Smoluchowskiego 17, 60-179 Poznań*

denitza_vladimirova@abv.bg

The search for suitable energy storage devices has been the subject of many investigations. Rechargeable zinc-air batteries are promising power sources that use inexpensive and environmentally benign materials. The high specific charge of zinc and oxygen electrodes offers the possibility to design batteries having exceptionally high specific energy. Recently much attention has been paid towards the development of efficient cathode catalysts. Development of efficient bifunctional catalysts, simultaneously active for oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), remains to be a biggest challenge.

The aim of the present work is to study oxide materials from $Ni_xCo_{3-x}O_4$ system, where x = 0.7, 1.4, 2.1 as potential bifunctional catalysts for oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). The materials are prepared by means of Pechini method and characterized by physical and electrochemical methods. The structural properties have been examined by X-ray diffraction, X-Ray Microtomography. Infrared spectroscopy, Differential thermal analysis. The XRD analysis shows that the oxides crystallize in a cubic spinel phase. The IR spectra are typical for cubic spinels with two bands of high intensity in the range 550 - 690 cm^{-1}. The electrochemical properties of the samples were studied by cyclic voltammetry elucidate the electrochemical behaviour of the samples.

The surface morphology is revealed by SEM image. They shows that the particles are mostly spherical in shape with size between 50 - 100 nm. Impedance investigations have been performed by using impedance spectroscopy at different temperatures.

POSTER - 28

THE CREATION OF STATIC ATOMIC DISPLACEMENT WAVES IN IRRADIATED $TlInS_2$ CRYSTALS

A. Nikolaienko[1], O. Zloi[1], M. Isaiev[1], Yu. Gololobov[2] and N. Borovoy[1]
[1]*Faculty of Physics, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
[2]*Department of Physics, National Transport University, Kyiv, Ukraine*
alina.salnik@gmail.com

$TlInS_2$ crystals (monoclinic modification) belongs to low-dimensional compounds $TlMX_2$ (M=Ga, In; X=Se, S, Te), which are a wide-band gap semiconductors and ferroelectrics with a layered structure. An important feature of these crystals is the existence of successive phase transitions (PT) which are accompanied by the formation of incommensurate (ICP) and commensurate (CP) phases in the temperature range 190 - 240 K. Additionally, layered crystals $TlInS_2$ characterized by a high concentration of defects of various types which significantly influences on the formation and properties of the ICP. The system of the defects can be changed by irradiating of the crystal with electrons and γ-radiation.

In our previous study it was observed the formation of modulated structures (ICP) in unirradiated crystals near 238 K with wave vector **q**(-δ, 0, +0.25) and **q**(+δ, 0, -0.25) (δ = 0.04) [1], and the increasing of the modulated satellites intensities at T = 214 K with further cooling. In presented work it was shown that after the irradiation of C-$TlInS_2$ crystals quite intensive satellites were observed even at room temperature. These satellites were more elongated in the a*-direction and without pronounced maxima. Thus, we can conclude that the irradiation the sample leads to the change of the points defect concentration. One may assume that in this case the fluctuations in the system of radiation-induced point defects lead to the formation of defect density waves (DDW). The DDWs, in turn, stimulate the creation of static atomic displacement waves. To verify this assumption molecular dynamics simulation of the simple two-dimensional square lattice (Fig. 1a) were carried out. It was shown on such a simple model [2] that the removal an atom from the lattice with subsequent relaxation on the vacancy leads to a static displacement waves (1b, 1c). On this model it was shown that the formation of the DDW can be accompanied by the appearance of static atomic displacements waves with different incommensurability parameter.

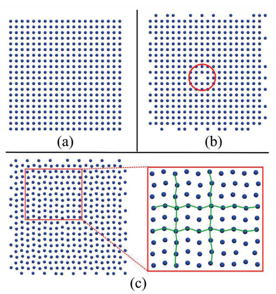

Fig. 1. The atomic displacements in the two-dimensional square lattice with defects.

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POSTER - 29

LIQUID CRYSTALLINE DERIVATIVES WITH TERPHENYL MOLECULAR CORE AND LACTIC ACID UNIT AS CHIRAL MOIETY

V. Novotná[1], V. Hamplová[1], G. Sasnouski[2] and P. Salamon[3]

[1]*Institute of Physics; Na Slovance 1999/2; 182 21 Prague 8, Czech Republic*

[2]*Institute of Applied Physics Problems, Kurchatova 7, Minsk 220045, Belarus*

[3]*Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, H-1121 Budapest, Konkoly Thege Miklos ut 29-33, Hungary*

novotna@fzu.cz

The terphenyl derivatives have been studied since the beginning of the liquid crystal research [1] and it has been established that they have great potential. Generally they exhibit rather high transition temperatures, which can be overcome by a lateral substitution. Very often fluorinated terphenyl derivatives were prepared and studied [2]. On the other hand, the mesomorphic properties are influenced not only by the character of the molecular core, but also by the character of linking groups and/or type of the chiral moiety. Lactic acid unit was often utilized in the chiral part for the synthesis of new liquid crystalline compounds [3]. Such derivatives exhibited good chemical and optical purity, thermal stability and their chirality is strong enough to promote the ferroelectricity.

Herein, new lactic acid derivatives, based on terphenyl molecular core laterally substituted by chlorine atom, have been synthesized and their liquid crystalline properties studied. We varied the molecular structure by prolonging the non-chiral chain and analyzed the mesogenic properties with respect to its length. We found that all studied compounds reveal the SmA*-SmC* phase sequence in an extremely broad temperature interval. The experimental techniques, namely the polarizing optical microscopy, differential scanning calorimetry, x-ray diffraction and helical pitch measurements, have been applied to establish the physical properties. Studied compounds exhibit very high values of the spontaneous polarization and the tilt angle grows continuously on cooling up to 42 degrees. The pitch values drop down when prolonging the molecular non-chiral chain.

In comparison with analogous lactic acid derivatives based on different molecular core [4] we can conclude that we reached broadening of the mesophase temperature interval down to the room temperatures.

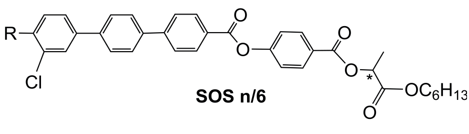

Fig. 1. Chemical formula of studied compounds designated as SOS n/6.

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POSTER - 30

PHYSICAL PROPERTIES OF PREPARED LIQUID CRYSTAL MIXTURES FORMING THE BLUE PHASES

K. Nowicka[1], M. Piosik[2] and W. Kuczyński[1]
[1]*Institute of Molecular Physic, Polish Academy of Sciences, Poznań, Poland*
[2]*Poznań University of Technology, Poznań, Poland*
kamila@ifmpan.poznan.pl

The blue phases (BPs) of chiral liquid crystals typically occur within a narrow temperature range between the chiral nematic and isotropic liquid phases [1-2]. Their origin has been ascribed to a competition between an intermolecular twist induced by chirality and the necessity of the molecules to fill space uniformly. This competition results in the mesogen self-organizing into double-twisted cylindrical structures that are separated by disclination lines. Three different network structures are known to form distinct blue phase morphologies with increasing temperature: these are denoted as blue phase I (BPI), blue phase II (BPII), and blue phase III (BPIII). In comparison to conventional nematic materials the blue phase exhibits several revolutionary features. First, it does not require any alignment layer, such as polyimide, which simplifies the manufacturing processes and reduces the cost. Second, the electro-optic response times, rise as well as decay time, are lower than 1 ms [3]. From an application viewpoint, blue phase liquid crystals with fast response are of interest for high speed light modulators, tunable photonics crystals, three-dimensional lasers, as well as new-generation displays. Many of these investigations are still at the exploratory and laboratory stage.

In this presentation, we will investigate the physical properties of the obtained liquid crystalline mixtures exhibiting BPs such as: (a) temperature range of occurrence of BP, (b) the number of BP phases or (c) grain size of typical mosaic texture of BPs. In order to obtain material exhibiting BPs the mixtures of selected nematic liquid crystals and chiral dopant will be prepared. Systematic study of chiral dopant in function of concentration in liquid crystals will be performed. Furthermore measurements in variable thickness of the sample for selected mixture will be presented.

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POSTER - 31

EFFECTIVE DIELECTRIC FUNCTION OF $BaTiO_3$-NiO NANO-COMPOSITES

D. Nuzhnyy[1], J. Petzelt[1], V. Bovtun[1], M. Kempa[1], P. Bednyakov[1], M. Savinov[1],
L. Fernández-Garciá[2], T. Rodriguez-Suarez[2] and J.L. Menendéz[2]
[1]*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*
[2]*Centro de Investigación en Nanomateriales y Nanotecnología (CINN), Consejo Superior de Investigaciones Científicas (CSIC), Universidad de Oviedo, El Entrego, Spain*
nuzhnyj@fzu.cz

Topology of composites plays an important role in the dielectric response of high-permittivity and highly absorbing materials with a strong dielectric contrast between the composite fractions.
We studied broadband dielectric response in the 10 - 700 K temperature range using Fourier-transform infrared reflectivity, time-domain THz transmission spectroscopy, high-frequency coaxial technique and standard low-frequency capacitance measurements of two types of composites of $BaTiO_3$ (BTO) with 30 vol% of NiO: core-shell BTO@NiO and standard topology composites. Both types of composites were processed using spark plasma sintering technique. The powder of BTO@NiO core-shell particles with ~200 nm BTO core and several nm NiO shell (Fig. 1) and standard powder of BTO and NiO with an average particle size of around 0.7 μm and 10 μm, respectively, were used to prepare the ceramic samples.
Experimental data were fitted to obtain the effective dielectric spectra in a broad frequency range and modelled using the effective medium approximation [1]. Dielectric spectra of the pure components of BTO and NiO were used from literature [2,3] to model the dielectric spectra of the composites using different effective medium approaches. At the same time, phonon dynamics and influence of the topology on the effective phonon behavior will be discussed.

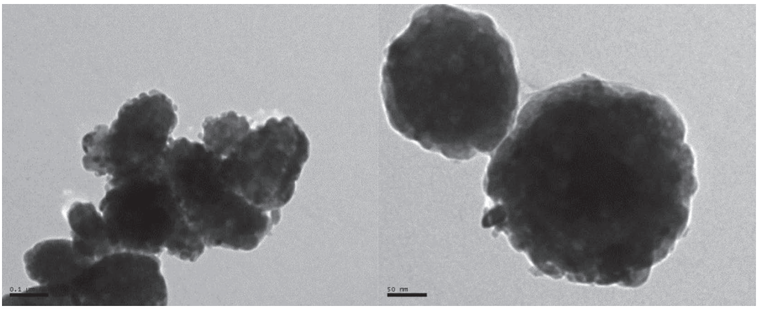

Fig. 1. Transmission electron microscopy images of $BaTiO_3$@NiO core-shell particles.

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POSTER - 32

POLARIZATION FLUCTUATIONS IN SBN SINGLE CRYSTALS

P. Ondrejkovic[1], M. Kempa[1], M. Savinov[1], J. Kulda[2], J. Dec[3] and J. Hlinka[1]
[1]Institute of Physics, The Czech Academy of Sciencies, Prague, Czech Republic
[2]Institut Laue-Langevin, Grenoble, France
[3]Institute of Materials Science, University of Silesia, Katowice, Poland
ondrejkovic@fzu.cz

One of the most interesting properties of $Sr_xBa_{1-x}NbO_3$ (SBNx) solid solution is the possibility of tuning its relaxor properties by variation of the Sr content. For example, the SBN61 concentration belongs to the most studied uniaxial relaxor ferroelectrics due to its enhanced dielectric and piezoelectric properties in the operating temperature region of electronic devices.
We intend to present neutron scattering studies of polarization fluctuations in SBN single crystals with enhanced relaxor properties. We will focus mainly on the diffuse scattering which is known to come from a very dense domain structure with 180-degree domain walls (see Fig. 1a) and from critical fluctuations in the phase transition region [1,2]. Both contributions give rise to a disk-like shape diffuse scattering (see Fig. 1b) at similar momentum transfers and therefore they are difficult to separate from the experimental data (Fig. 1c, d). However, they show different temperature dependences and distinct changes under the bias electric field [1]. We will discuss the behaviour of these two contributions under electric field and thermal treatments and compare them to dielectric measurements.

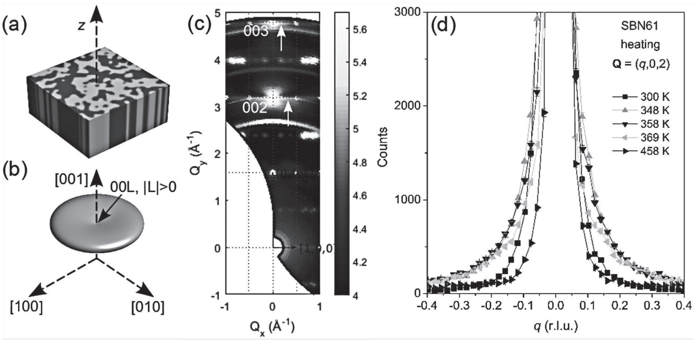

Fig. 1. Sketches (a) and (b) indicate a typical nanodomain structure of a uniaxial relaxor and the equi-intensity surface of the associated diffuse scattering. Example of this transverse diffuse scattering (c) in an intensity map of elastic scattering (indicated by arrows) at 380 K in SBN50 on IN20 and (d) in elastic scans at Q = (q,0,2) in SBN61 single crystal on IN3 ILL, Grenoble.

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POSTER - 33

UNIVERSALITY OF CONDUCTIVITY SPECTRA IN SUPERPROTONIC $(NH_4)_3H(SO_4)_2$ SINGLE CRYSTAL

Cz. Pawlaczyk, A. Pawłowski and P. Ławniczak
Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
czpawl@ifmpan.poznan.pl

Frequency dependencies of conductivity $\sigma^*(\omega)$, $[\sigma^*(\omega) = \sigma'(\omega) - \sigma''(\omega)]$ of the most common disordered ion conductors show an universal frequency response, the so-called first and second universalities [1,2]. The first universality is related to the thermally activated hopping mechanism of ionic migration (conductivity) through solid state in microscopic scale whereas the second universality, often called Nearly Constant Loss (NCL) effect, is the effect observed at sufficiently low temperatures or in a range of high frequencies. In such conditions the translational movements of ions through solid state do not contribute to dielectric loss.

In this contribution we presents the results of conductivity measurements for single crystalline $(NH_4)_3H(SO_4)_2$ (AHS) in crystallographic a direction. This crystal belongs to family of crystalline proton conductors which undergo a phase transition from low (at lower temperatures) to high conductivity phase (at higher temperatures). The AHS crystal undergoes superprotonic phase transition at 413 K. Fig. 1a shows the temperature dependence of DC conductivity (Arrhenius plot) whereas in Fig. 1b the master curve for the low conducting phase is presented.

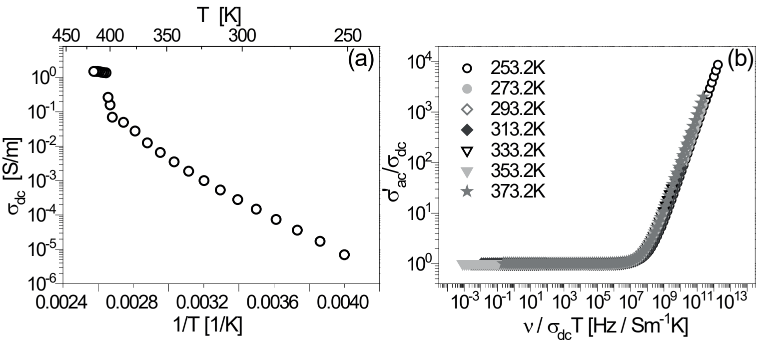

Fig. 1. Arrhenius plot of AHS along a direction (a). Master curve of the real part of conductivity for AHS in low conducting phase (b).

We prove that conductivity spectra of $(NH_4)_3H(SO_4)_2$ show in the low conducting phase similar universal features as common disordered solid state ionic conductors.

Acknowledgment
This work is supported by Polish National Science Centre under grant No. 2014/15/D/ST3/03433.

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POSTER - 34

IMPEDANCE SPECTROSCOPY STUDY OF $(NH_4)_3H(SeO_4)_2$: EVIDENCE OF INCREASE IN LATTICE DISORDER IN THE LOW TEMPERATURE PHASES

Ł. Lindner, M. Zdanowska-Frączek, **A. Pawłowski**, Z. Frączek
Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
antoni@ifmpan.poznan.pl

$(NH_4)_3H(SeO_4)_2$ belongs to the group of hydrogen bonded crystals of general formula $M_3H(XO_4)_2$, where M = NH_4, Rb, K, Cs and X = S, Se. All the crystals undergo structural superionic phase transitions at elevated temperatures. Above superionic phase transition temperature T_S the proton conductivity reaches values up to ~10^{-2} S/cm with activation energy E_a = 0.30 - 0.60 eV, depending on the crystal formula and the direction.

The ammonium salt shows a rich sequence of phase transitions. The two high temperature phases I and II, in descending order of temperature, are trigonal ($R\overline{3}m$ and $R\overline{3}$, respectively) and exhibit a high proton conductivity. The fast proton diffusion in the phases I and II is conditioned by an excess of structurally equivalent positions for protonic charge carriers in the crystal lattice combined with a high molecular dynamics. Although the low temperature phases do not comprise excess positions for protons, their proton conductivity is relatively high and an increasing molecular dynamics is observed on heating far below phase III-II transition temperature T_{S2} = 300 K. In order to evidence the build up of molecular dynamics as temperature approaches T_{S2} we present here the results of electric impedance measurements of $(NH_4)_3H(SeO_4)_2$ along the monoclinic c* axis. We studied dielectric properties of the phases IV and III over a wide range of frequency and temperature. The presented findings give a new insight into the evolution of molecular dynamics and its relation to proton transport mechanism.

It is known, that the frequency dependence of conductivity follows the Jonscher's universal dynamic law $\sigma(\omega) = \sigma(0) + A\omega^s$. The obtained s values vary slightly in a narrow range between 0.40 and 0.45 in the monoclinic (space group C2/c) ferroelastic phase IV (below T_{IV-III} = 273 K) and point to the hopping mechanism of proton conductivity. The behavior of the exponent changes considerably in the ferroelastic triclinic ($C\overline{1}$) phase III, where it decreases stepwise at T_{IV-III} and lessens rapidly with increasing temperature to reach a value close to zero at T_{S2}. Such behavior points to an appreciable increase in lattice disorder when approaching the superionic phase. In other words the intermolecular interactions in the lattice become increasingly averaged as temperature approaches T_{S2}.

The electric modulus formalism was used to the analysis of electric relaxation in $(NH_4)_3H(SeO_4)_2$. The frequency dependence of the imaginary part M″ of the electric modulus M* shows asymmetric peaks which shift toward higher frequency with temperature. The frequency at each peak position separates frequency range of a long distance proton transport (below) and localized motion (above). Similar behavior is observed in both phases IV and III, but the peaks are higher in the phase III. The conductivity relaxation times τ were derived from the condition $2\pi f_{max}\tau = 1$, where fmax is the frequency at the peak position. Reciprocal temperature plot of τ shows the Arrhenius behavior $\tau = \tau_0 \exp(E/kT)$ in both phases with the exception of the high temperature end of the phase III (close to the superprotonic phase), where a rapid decrease in τ is observed. The calculated activation energies of τ are 0.36 eV in the phase IV and 0.82 eV in the phase III and agree satisfactorily with the values obtained from the conductivity measurements.

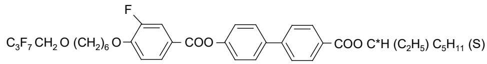
POSTER - 35

DIELECTRIC PROPERTIES OF NEW FLUORINATED COMPOUNDS EXHIBITING FERRO- AND ANTIFERROELECTRIC PHASES

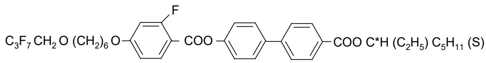
P. Perkowski and M. Żurowska
Military University of Technology, Warsaw, Poland
pawel.perkowski@wat.edu.pl

Four newly synthesized at MUT ferroelectric liquid crystals were investigated be means of dielectric spectroscopy. All compounds exhibit para- and ferroelectric phases, while compound 1 shows also wide-temperature antiferroelectric phase.

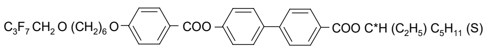
Compound 1



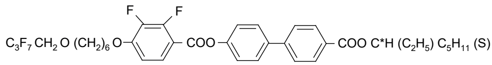
Compound 2



Compound 3



Compound 4



Investigated compounds show interesting dielectric properties. Fig. 1 shows that for compound 1 it is difficult to define the temperature of phase transition SmC* - SmC$_A$*. It is good example of confirmation that this phase transition is the second order one. Results for other compound are shown and discussed. 10 V DC field is enough to suppress Goldstone mode. Soft mode in SmA* becomes visible. Surprisingly only PH mode is observed in SmC$_A$* while PL mode is not detectable.

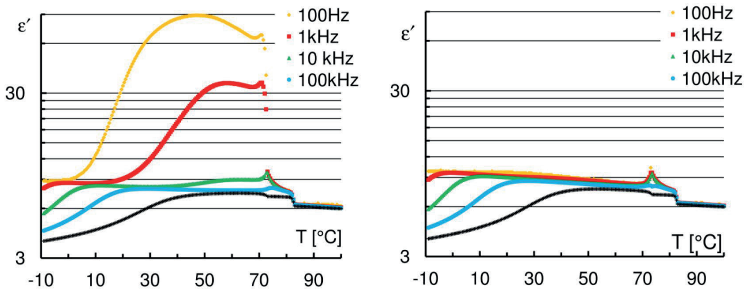


Fig. 1. Real part ε' of electric permittivity for compound 1 versus temperature at five frequencies of measuring field (100 Hz, 1 kHz, 10 kHz, 100 kHz, 1 MHz). Left - no DC field, right - 10 V DC field.

Investigations supported by University grant PBS 23-652.

POSTER - 36

STRUCTURAL AND ELECTRICAL FEATURES INDUCED BY LEACHING PROCEDURES ON $LiNbO_3$ CRYSTALLINE POWDER SAMPLES

J. Piecha[1], M. Dabioch[2], A. Leonarska[1]
[1]*Institute of Physics, University of Silesia, 40-007 Katowice, Poland*
[2]*Institute of Chemistry, University of Silesia, 40-006 Katowice, Poland*
julita.piecha@us.edu.pl

The crystalline powders of congruent lithium niobate were studied. Measurements were carried out on pure (reference) powder and powders modified by leaching procedure. Leaching reactions were conducted at redistilled water and at concentrated nitric acid at temperature of 80 °C for 48 h each. Reaction carried out in nitric acid environment led to proton exchange Li^+/H^+ [1]. The concentration of lithium and niobium in liquid solutions was determined using an optical emission spectrometry with excitation by argon inductively coupled plasma (ICP-OES). The X-ray powder diffraction (XRD) test was performed to verify the stability of crystallographic structure of the powders of $LiNbO_3$ [2] affected by the leaching procedure. The ICP-OES and XRD measurements were conducted at room temperature. For leached powder sample, the intensity of diffractogram pattern was significantly lower than the intensity obtained for the reference powder sample, however the space group *R3c* was maintained. Electrical studies were carried out to check the influence of leaching reaction on electric permittivity and loss coefficient tanδ [3,4]. The spectra were obtained for frequency range from 20 Hz to 1 MHz, measurements were conducted at temperature range from 300 K to 600 K.

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POSTER - 37

INFLUENCE OF THERMAL TREATMENT ON PROPERTIES OF $BiMnO_3$ CERAMICS

M. Pilch and A. Molak
Institute of Physics, University of Silesia, Katowice, Poland
michal.pilch@us.edu.pl

We have developed the means to sinter $BiMnO_3$ in N_2 flow. The X-ray diffraction test has indicated occurrence of two phases with monoclinic and centrosymmetric symmetries. Grain structure and stoichiometry has been observed by scanning electron microscopy whereas local disorder by X-ray photoemission spectroscopy. We have described the role of N-induced modification of band gap assigned as O2p, Mn 3d charge transfer, with some addition of Bi 6p states. Electric conductivity has been measured in the 100 - 770 K range. The electric impedance measurements show marked dispersion. The studied fresh ceramics confirm semiconductor properties.

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POSTER - 38

SPECTRAL INVESTIGATIONS OF PROTON CONDUCTING MATERIAL $(IMD)_2SeO_4{\cdot}2H_2O$

S. Zięba, A. Mizera, A. Łapiński and **K. Pogorzelec-Glaser**
Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland
kglaser@ifmpan.poznan.pl

In this work, the vibrational properties of imidazolium selenate dihydrate crystals will be presented and discussed. In this system, the SeO_4 ions form a hydrogen bond network and protons can effectively diffuse through the network at high temperature in the superprotonic phase. The selenate anions SeO_4^{2-} have slightly distorted tetrahedral geometry and together with the water molecules form the three dimensional network with the strong hydrogen bonds of the O-H…O type. The imidazole cations are almost flat and exhibit the characteristic deformation of the heterocyclic ring from pentagonal form [1].
In our investigations we used IR and Raman spectroscopy, supported by DFT calculations. Raman spectra were recorded with the excitation line λ = 514 nm on a Jobin-Yvon HORIBA LabRAM HR 800 spectrometer. The FT-IR absorption spectra of imidazolium selenate dihydrate were measured in KBr pellets (c = 1:2000) in the range between 400 and 7500 cm^{-1} using a FT-IR Bruker Equinox 55. We have performed the quantum-chemical calculations of normal modes with the Gaussian 03 sets of codes. The B3LYP hybrid density functional and 6-311++G(d,p) basis sets were used. The initial geometry in optimization process was taken from X-ray data [1].
In the Raman and IR spectra of imidazolium selenate hydrate, the most intensive bands observed at 1224, 1463, and 1597 cm^{-1} are related to the imidazole cation. The last mode is due to the stretching C=C bonds within a pentagonal ring, whereas the other bands are mainly due to the carbon-nitrogen stretching vibrations. In our theoretical considerations we assumed that in our system we could have SeO_4^{2-} anions with T_d symmetry, $HSeO_4^-$ ion with C_{3v} or C_1 symmetries, and/or H_2SeO_4 with C_1 symmetry. Such assumption may be justified because in our system we have distorted selenate anions caused by interactions with the neighbouring hydrogen atoms. Taking into account theoretical predictions we could give the interpretation of our experimental data. The bands at 1124, 1052, 913, 640 cm^{-1} are assigned to H_2SeO_4, the bands observed at 1094, 882, 849, 826, 415 cm^{-1} are assigned to $HSeO_4^-$ ion, whereas bands at 804, 794, 440, 336 cm^{-1} are due to SeO_4^{2-} ions. These results show that for $(IMD)_2SeO_4{\cdot}2H_2O$ the high mobility of protons is present. In the investigated crystal the OH stretching absorption bands reveal the characteristic ABC structure expected for short hydrogen bonds, with maxima at approximately ~2800 cm^{-1} (A), ~2600 cm^{-1} (B), and ~1900 cm^{-1}(C). Such structure may be explained on the basis of Fermi resonance between the OH stretch, the overtone 2γOH and the combination βOH+γOH [2]. The bands at about 980, 590 cm^{-1} in IR spectrum can suggest that hydronium ions H_3O^+ [3] is present in our compound.

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POSTER - 39

XRD, RAMAN AND MAGNETIC STUDIES OF $Bi_{1-x}La_xFeO_3$ SOLID SOLUTION OBTAINED BY MECHANOCHEMICAL SYNTHESIS

M. Połomska[1], B. Hilczer[1], I. Szafraniak-Wiza[2], A. Pietraszko[3] and B. Andrzejewski[1]

[1]*Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland*

[2]*Institute of Materials Science and Engineering, Poznań University of Technology, Poznań, Poland*

[3]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland*

polomska@ifmpan.poznan.pl

Bismuth ferrite, interesting for applications in information storage and sensors, exhibits antiferromagnetic properties below $T_N \approx 640$ K and is ferroelectric below $T_C \approx 1100$ K [1-3]. The temperature T_C was found to be shifted downwards in $BiFeO_3$-$LaFeO_3$ solid solution, which is expected to increase the magneto-electric coupling [4]. As a decrease in the particle size below the periodicity of cycloid modulation (62 nm) can modify the magnetic properties we studied the properties of $Bi_{1-x}La_xFeO_3$ nanosize powders produced by mechanical synthesis.

The Bi_2O_3, Fe_2O_3, La_2O_3 oxides (Aldrich, 99% purity) of weight ratio corresponding to the x value were mechanically activated in a SPEX 8000 Mixer Mill at room temperature in the air. The weight ratio of the stainless steel balls to the oxides was 2:1. The synthesis was controlled by XRD and the powder was characterized by TEM and NIR Raman spectroscopy. Magnetic properties were measured with Quantum Design PPMS System. The powders obtained after 120 h milling of the oxides were found to exhibit rhombohedrally distorted perovskite structure and TEM observations show that the powder forms irregular 100 - 150 nm loosely packed agglomerates of oval 10 - 30 nm grains. The nanograins exhibit core-shell structure with crystalline core surrounded by a disordered shell (1 - 2 nm thick). Thermal treatment (1 h at 500 °C) results in a disappearance of the shell and an increase in the grain size to 40 - 50 nm.

FT NIR Raman spectra of as synthesized nanopowders are characterized by broad bands. Crystallization of the shell is observed as band narrowing and the structure of the spectra becomes richer. The nanopowders of $Bi_{1-x}La_xFeO_3$ solid solutions with core-shell structure of the grains were found to exhibit field-dependent $\chi(T)$ anomaly at ~ 8 K in ZFC measurements, whereas a continuous increase in the χ values was observed down to 2 K in FC-experiments. Magnetic hysteresis loops were observed for the compounds both as-prepared and annealed. The magnetization loops were not really saturated which points to basic antiferromagnetic nature and the annealing was found to decrease the magnetization considerably. The improvement of magnetization in nanosize particles obtained by mechanical activation we would like to relate both to lack of spin compensation in the cycloid along the direction of the wave vector and an increase in the spin canting due to the stress extended by the grain shell resulting in ferromagnetism.

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POSTER - 40

FLEXIBLE CRYSTALS OF PEROVSKITE-LIKE COORDINATION POLYMERS WITH TUNABLE AND SWITCHABLE ORGANIC GUEST

J.K. Prytys[1], M. Rok[1], V. Kinzhybalo[2] and G. Bator[1]
[1]*Faculty of Chemistry, University of Wroclaw, Joliot-Curie 14, 50-383 Wroclaw, Poland*
[2]*Institute of Low Temperature and Structure Research, Polish Academy of Science, Okólna 2, PO Box 937, 50-950 Wroclaw, Poland*
joanna.prytys@chem.uni.wroc.pl

A family of the cyano-bridged coordination polymers (CPs), which undergo transition between high and low dielectric state upon thermal stimulus, are promising materials with potential application in electrical and electronics devices. The good examples of such materials are crystals with perovskite type structure, where the organic-inorganic hybrids with the general formula RMX_3 (where R - organic cation, M - metal, X - halogen atom) have the same crystal structure like perovskite $CaTiO_3$. The best known compound from this group is the crystal of methylammonium iodoleadate ($MAPbI_3$), which was applied in the photovoltaic, show extraordinary large efficiency of a conversion of the solar light into electric energy, even exceeded that of the silicon systems of the mixed inorganic semiconductors. The carefully designed cage compounds with organic quest molecules as cations, may give materials where solid-to-solid phase transitions, with different nature, like order-disorder or displacive-type, can be observed. However, quests should have relatively small dimensions, a spherical form and be endowed with a dipole moment in order the dynamical effects could be observed. Moreover, the switchable quest cations into the well-matched anionic host framework should possess a relatively large freedom for rotation, i.e. they should have the possibility to jump between at least two positions energetically equivalent. The reorientation of the polar quest may result in a switch of the polarization. The molecular dynamics affects the dielectric constant, non-linear optics, magnetic susceptibility. Recently, the CPs crystal of $K_3Fe(CN)_6$ with methyl derivatives of amine cation as quest molecule has been investigated [1]. The electric studies concerned however a polycrystalline form of the compound. Encouraged by these pioneering studies we would like to report the result on the dielectric parameters for the single crystals $(CH_3NH_3)_2KFe(CN)_6$. On the basis of these parameters the dynamics model of the cationic motions will be proposed. The detailed analysis of the structural properties would allow us to describe a correlation between the microscopic structure and the dielectric and optical properties of crystals.

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POSTER - 41

AVALANCHE CRITICAL EXPONENTS IN NANOPOROUS SYSTEMS UNDER COMPRESSION

S. Puchberger[1], V. Soprunyuk[1], W. Schranz[1], A. Tröster[2], E. Vives[3] and E.K.H. Salje[4]
[1]*Faculty of Physics, University of Vienna, Vienna, Austria*
[2]*Institute of Material Chemistry, Vienna University of Technology, Vienna, Austria*
[3]*Department d'Estructura I Constituents de la Matéria, Universitat de Barcelona, Barcelona, Spain*
[4]*Department of Earth Science, University of Cambridge, Cambridge, United Kingdom*
a1047730@unet.univie.ac.at

This study investigates the behavior of nanoporous materials under compression. Some porous materials respond to the application of an external force in a sequence of jerky events (avalanches) due to the correlated collapsing of nanometer-scaled pores. These avalanches show scale-invariance and appear in broad size distributions (power-laws). It has been discovered that such jerky events are independent of both the macroscopic and microscopic details of the systems [1] and, therefore, the critical exponents of such power-laws are universal. In order to study universality and derive values for critical exponents renormalization group methods are used. Crackling exhibits many similarities to phase transitions near the critical point and tools that are usually employed to study phase transitions are useful in investigating crackling behavior as well.
The measurement technique involves an analysis of strain drops with a Diamond DMA (Dynamical Mechanical Analyzer, PerkinElmer) at slowly varying compressive stress (0.1 mN/s - 10 mN/s). The samples selected were on the one hand Gelsil and Vycor, both SiO_2-based synthetic materials, which have been studied previously with acoustic emission and, on the other hand, Shale which is a natural porous sedimentary rock. The jerky evolution of the sample's height with time is analyzed in order to determine the corresponding power-law exponents for the maximum velocity distribution, the squared maximum velocity distribution as well as the aftershock activity in the region before macroscopic failure. A comparison with recent results from acoustic emission data on the same materials [2] shows similitude in the statistics, although the two methods operate on different spatial and temporal scales. Moreover, the obtained power-law exponents are in reasonable agreement with theoretical mean-field values [3].

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POSTER - 42

BASIC CHARACTERIZATION AND STANDARD DIELECTRIC MEASUREMENTS ON PLZT x/65/35 CERAMICS BASED ON CORRELATION COEFFICIENTS

K. Pytel[1], J. Suchanicz[1], W. Hudy[1], M. Livinsh[2] and A. Sternberg[2]
[1]*Institute of Technology, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*
[2]*Institute of Solid State Physics, University of Latvia, Kengaraga 8, LV-1063 Riga, Latvia*
kpytel@up.krakow.pl

The influence of external stress (< 800 bar) on the dielectric properties of PLZT x/65/35 (2?x?13) ceramics was investigated. The high density of the PLZT x/65/35 (x=2, 4, 6, 7, 9.75, 10, 11 and 13) ceramics with the average grain size of ca. 5 - 8 μm was obtained by the two-stage hot-pressing technology. Applying uniaxial pressure leads to a change in the peak intensity of the electric permittivity of its frequency dispersion as well as in the dielectric hysteresis. Results based on nanoregion switching processes under combined electromechanical loading were interpreted.

A correlation between the experimental data was determined. A counted correlation coefficients illustrated a quantitative measure of some type of correlation and dependence. Types of correlation coefficients included Pearson product-moment correlation coefficient and Spearman's rank correlation coefficient. A Kolmogorov Smirnov test was used to compare results.

Surveys demonstrated that applied stress has a significant influence on the dielectric properties of PLZT ceramics.

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POSTER - 43

DYNAMICS OF COLLECTIVE MODES IN FERROELECTRIC LIQUID CRYSTAL GELS

S.A. Różański
Stanisław Staszic University of Applied Sciences in Piła, Piła, Poland
srozansk@asta-net.com.pl

Liquid crystal gels are attractive kind of functional materials characterized by new electro-optical, dielectric and other physical properties which can be used in display technology [1-4]. Usually the gel-former agent is dissolved in liquid crystal and can form a hydrogen-bonding network in the liquid crystal host [1]. This network can be destroyed by heating and associated by cooling of the system. Some gelators can be switched by UV-light from *trans* to *cis* conformation which has an impact on the switching time in FLC-gel systems [4].

In the present study, broadband dielectric spectroscopy (BDS) was applied to investigate the dynamics of the soft mode and the Goldstone mode in a pure ferroelectric liquid crystal mixture (FLC13 Clariant) and FLC13 containing some weight percent of organic gel-forming agent PD4HG [4]. In the bulk FLC13 the dynamics of collective relaxation processes shows characteristic features: i) the soft mode present in the SmA phase splits into the Goldstone mode and the soft mode in the SmC* ferroelectric phase, ii) the characteristic frequency of the soft mode in the SmA phase decreases and in the SmC* phase increases with decreasing temperature but the dielectric strength increases in the SmA phase and decreases in the SmC* phase, iii) the Goldstone mode in the SmC* phase masks the rather weak soft mode and can be suppressed by an electric field. The characteristic frequency of the Goldstone mode is nearly temperature independent.

After adding PD4HG gelator to the FLC13, the dielectric measurements were performed on the fresh samples, after annealing in proper temperature and after heating above the gelation point. BDS measurements show that dynamics of the Goldstone mode is altered by the presence of gel-former hydrogen-bonded structure in the FLC13. The dielectric relaxation strength of the Goldstone mode changes with the gel-former concentration and thermal treatment of the FLC-gel samples, which can be related to differences in the gel structure created in FLC13. Some molecules participating in the fluctuation of the azimuthal angle on the cone can be immobilized by the hydrogen-bonded gel network which causes a decrease of the Goldstone mode dielectric strength.

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POSTER - 44

RELATIONSHIP BETWEEN DIELECTRIC AND ELASTIC PROPERTIES OF THE POROUS CERAMICS

I. Rychetsky and A. Klic
Institute of Physics, ASCR, Czech Republic
rychet@fzu.cz

The problem of cross-property connection between physical quantities of different origin is of great interest in various fields of material science, particularly in cases when various properties are not known or difficult obtainable, while others can be more easily measured. In porous materials these can be, e.g., electrical conductivity, fluid permeability, mechanical properties represented by the Young's modulus, porosity, etc. The overall macroscopic properties and their interrelationships depend on the micro-structural parameters such as volume fractions of components, shapes and distribution of grains and pores, and general treatment of this problem is considerably complex [1-3].
In this contribution we study the model, which was previously successfully used to describe the dielectric properties of the porous perovskite ceramics PMN. Using the finite element analysis the effective dielectric and elastic properties of the samples with several porosities is calculated. Numerically obtained dependences of the Young's modulus and permittivity on the so-called percolation strength (i. e., electrical structural parameter) is compared with various existing formulas [3].

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POSTER - 45

BROADBAND DIELECTRIC SPECTROSCOPY OF THE NON-RELAXOR $PbFe_{1/2}Ta_{1/2}O_3$ CERAMICS

M. Savinov[1], P. Bednyakov[1], S. Skiadopoulou[1], F. Kadlec[1], V. Bovtun[1], M. Kempa[1], A.A. Gusev[2], I.P. Raevski[3], V.P. Isupov[2], S.I. Raevskaya[3], M.A. Malitskaya[3], V.V. Titov[3], H. Chen[4] and S. Kamba[1]

[1]*Institute of Physics, AS CR, Prague, Czech Republic*

[2]*Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Kutateladze 18, Russia*

[3]*Research Institute of Physics, Southern Federal University, Rostov on Don, Russia*

[4]*Institute of Applied Physics and Materials Engineering, Faculty of Science and Technology, University of Macau, Macau, China*

savinov@fzu.cz

$PbFe_{1/2}Ta_{1/2}O_3$ (PFT) belongs to the rich family of double perovskites $Pb(M'^{3+}_{1/2}M''^{5+}_{1/2})O_3$ with M'=Fe, Sc, In, Yb, and M"=Nb, Ta, Sb. In these compounds, M'^{3+} and M''^{5+} cation positions may be either ordered or disordered. As a rule in the ordered state these perovskites have non-diffused ferroelectric or antiferroelectric phase transitions while in the disordered state they exhibit a relaxor behavior [1]. Recently we found out [2] that in contrast to PFT single crystals [3] and ceramics obtained by a routine solid state reaction route [4], PFT ceramics sintered from mechanoactivated powders do not show relaxor properties in the 102-106 Hz frequency range though Fe and Ta cations are disordered.

In the present contribution, complex dielectric permittivity of the PFT ceramics sintered from mechanoactivated powders were obtained in the low-frequency (1 Hz - 1 MHz), microwave (1 MHz - 1.8 GHz), THz (100 - 500 GHz) and infrared (1 - 100 THz) regions. PFT undergoes phase transitions from the cubic paraelectric ($Pm\bar{3}m$) to tetragonal ferroelectric (*P4mm*) phase at T_{C1} = 240 - 270 K, and then to the monoclinic ferroelectric (*Cm*) phase, at T_{C2} = 200 - 220 K [5]. Both ferroelectric phase transitions are revealed in the temperature change of permittivity and pyroelectric current. Measurements of polarization hysteresis loops revealed a well defined ferroelectric behavior with saturated polarization up to 15 $\mu C/cm^2$ ($E_c \sim 20$ kV/cm at 50 K) and a remnant polarization appearing below ≈ 280 K.

THz and far IR studies revealed hardening and splitting of the soft mode below T_{C1}. Additional heavily damped phonon is seen below the soft mode frequency. The same mode is well known in all relaxor ferroelectrics [6]. Its origin will be discussed.

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POSTER - 46

ON THE BEHAVIOUR OF LIQUIDS AND POLYMERS IN NANO-CONFINEMENT

V. Soprunyuk, M. Reinecker and **W. Schranz**
University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria
wilfried.schranz@univie.ac.at

Materials confined in nano-scale geometries exhibit very rich physics [1] and are interesting not only from the fundamental point of view, but they are of increasing importance for nanotechnology applications. Size effects play an important role at structural phase transitions, melting transitions, in martensitic materials [1], glass transitions, etc. Very often the question arises, whether a measured size effect originates from the confinement itself, or if it appears due to the interaction with the limiting surface. Using Dynamical Mechanical Analysis (DMA) technique we have studied various molecular glass forming liquids [2] as well as supercooled water [3] confined in nanoporous silica and phase segregated polymers [4]. We show on various examples that DMA measurements can help to disentangle bulk and surface effects in many important systems, including even freezing of water in biological materials (Fig. 1).

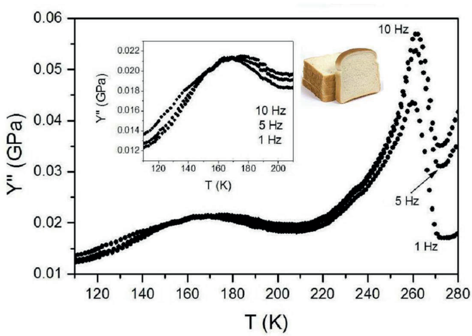

Fig. 1. Temperature and frequency dependence of the imaginary part of Young´s modulus of white bread. White bread contains approx. 38% of water and exhibits a similar freezing scenario as water in Vycor [3].

Acknowledgements
The present work was supported by the Austrian Science Fund (FWF, project Nr. P 28672 - N36).

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POSTER - 47

ORIENTATIONAL FLUCTUATIONS AND PHASE TRANSITIONS IN 8CB CONFINED BY CYLINDRICAL PORES OF PET FILM

G.I. Maksimochkin[1], **D.V. Shmeliova[1]**, S.V. Pasechnik[1], A.V. Dubtsov[1], O.A. Semina[1] and S. Kralj[2]

[1]*Moscow Technological University (MIREA), Moscow, Russia*

[2]*University of Maribor, Maribor, Slovenia*

shmeliova@mail.ru

The results of optical investigations of isotropic - nematic (I-N) and nematic-smectic A (N-A) phase transitions in porous polyethyleneterephthalate (PET) films filled with octyl-cyanobihenyl (8CB) are presented. The samples of porous films of a thickness 23 μm with normally oriented cylindrical pores of a radius R ranging from 10 nm to 1000 nm were prepared by the well-known technology of production of track-etched membrane. Dynamic light scattering method [1] was used to study orientational fluctuations of a liquid crystal at strong confinement. The relaxation rate τ of the orientational fluctuations as functions of the radius and temperature were determined. The latter dependence was obtained at slow cooling (0.3…0.6 K/h) which is needed for correct determination of the transition temperatures [2]. The example of $\tau(T)$ dependence presented in Fig. 1 (left) demonstrates the high sensitivity of this parameter to the phase transformations in liquid crystals. The dependences of I-N and N-A phase transition's temperatures on a pore radius are shown in Fig. 1 (right). The obtained results are analyzed in the frame of Landau-type phenomenological approach and compared with the results of calorimetric studies of 8CB confined to controlled-pore glass [2].

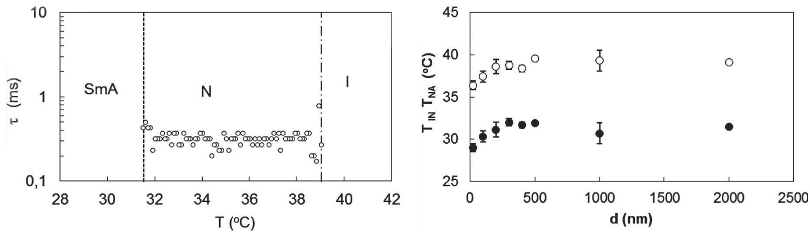

Fig. 1. Temperature dependence of relaxation rate τ for d = 400 nm and dependences of I-N (○) and N-A (●) phase transition's temperatures on a pore diameter.

Acknowledgements

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POSTER - 48

EFFECT OF UNIAXIAL STRESS ON THE DIELECTRIC PROPERTIES OF $BaTiO_3$+0.1% Eu CERAMICS

D. Sitko[1] and J. Suchanicz[2]

[1]*Institute of Physics, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*

[2]*Institute of Technology, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*

dsitko@up.krakow.pl

$BaTiO_3$+0.1%Eu ceramics were prepared by solid-state reaction method. The dielectric behavior of these ceramics as a function of uniaxial pressure has been systematically studied. The external stress showed obvious effects on these properties. An increase of the Curie point (T_C) and decrease of the Curie-Weiss temperature (T_0) was observed with increasing pressure, resulting in an increase in the first order nature of the phase transformation (T_C - T_0 decreases). The broadening and flattening of the permittivity versus temperature curves near their maximum were found. This could be ascribed to the inducing of non-ferroelectric cubic islands in the tetragonal phase by the applied compressive stress. On the other hand the pressure behavior of thermal hysteresis and the $\partial\varepsilon/\partial T$ vs. T plot strongly suggests that the phase transition changes to second-order type with increasing pressure. The Curie-Weiss constant obtained from a modified Curie-Weiss law strongly decreases with increasing pressure, suggesting that the mechanism of phase transition is going to order-disorder type. An increase in the difference between the Curie T_C and Burn's T_B temperatures with increasing pressure is observed, resulting in an narrowing of the temperature range on which the Curie-Weiss law is valid. Some kind of relaxation near T_C, which is strongly coupled with strain caused by applied compressive stress, is postulated. In general, the obtained results are similar to these obtained for pure $BaTiO_3$.

POSTER - 49

HIGH TEMPERATURE STUDY OF $LiNaSO_4$

Z. Slavkova[1], O. Koleva[1], P. Ławniczak[2], Ł. Lindner[2], M. Zdanowska-Frączek[2] and T. Petkova[1]

[1]*Institute of Electrochemistry and Energy Systems, BAS, Acad. G. Bonchev bl. 10, 1113 Sofia, Bulgaria*

[2]*Institute of Molecular Physics, PAS, Smoluchowskiego 17, 60-179 Poznań*

zdravka_slavkova@abv.bg

The increased energy demand of our society forces ecological power sources development. The lithium ion batteries are among the most used devices in consumer electronics. Wide application is due to their advantages: (i) lightweight; (ii) high working voltages resulting in high capacity; (iii) wide temperature range; (iv) quick charging; (v) long cycle life. The traditional electrolytes in lithium batteries which consist of organic lithium salts often are the reason for problems like formation of interphase and irreversible capacity losses, limit in the working temperature and decrease of the lithium batteries safety. By using solid state electrolyte one can overcome most of the problems. The search of new materials with properties suitable for an electrolyte is an essential scientific task.

The $LiNaSO_4$ is a promising candidate due to the existence of high temperature phase which ordinarily is highly ion conductive.

The present work deals with temperature study of $LiNaSO_4$ aiming to derive the correlation between the structure modification and electrochemical behaviors.

The samples are synthesized mechano-chemically for 8, 24, 52 and 72 hours. The results of X-ray analysis at ambient temperature shows only phase of $LiNaSO_4$ in all prepared samples.

A high temperature X-ray analysis is performed using Empyrean instrument supplied with special software and high temperature appliance. The stepwise heating and phase determination at the every temperature stage of the experiment reveal the existed phases and the percentage of each phase. The expansion thermal coefficient is calculated from the X-ray data. The transition from β to the highly conductive α phase is observed at about 540 °C. The results display that the process of transition is completed at 580 °C.

The increase of conductivity above 540 °C measured by high temperature impedance analysis confirms the appearance of high conductive phase.

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POSTER - 50

DIELECTRIC, THERMAL AND RAMAN PROPERTIES OF LEAD-FREE $(Na_{0.5}Bi_{0.5})_{1-x}Sr_xTiO_3$ (x=0, 0.04 and 0.06) CERAMICS

J. Suchanicz[1], V. Bovtun[2], E.M. Dutkiewicz[3,4], K. Konieczny[1], D. Sitko[3], K. Kluczewska[1], A. Wajda[5], M. Antonova[6] and A. Sternberg[6]

[1]*Institute of Technics, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*

[2]*Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Prague 8, Czech Republic*

[3]*Institute of Physics, Pedagogical University, ul. Podchorazych 2, 30-084 Krakow, Poland*

[4]*Institute of Nuclear Physics PAN, ul. Radzikowskiego 152, 31-342 Krakow, Poland*

[5]*Faculty of Materials Science and Ceramics, AGH-University of Science & Technology, al. Mickiewicza 30, 30-059 Krakow, Poland*

[6]*Institute of Solid State Physics, University of Latvia, LV-1063 Riga, Latvia*

sfsuchan@up.krakow.pl

Lead-containing ceramics based on the solid solution $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) have been dominating the markets of electronic devices due to their excellent piezoelectric performance [1]. However, the toxicity of lead has raised serious environmental pollution. This makes the search for lead-free replacement for PZT. $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) and NBT-based compounds recently became attractive as an alternative to lead-containing electronic materials [2].

Lead-free $(Na_{0.5}Bi_{0.5})_{1-x}Sr_xTiO_3$ (x=0, 0.04 and 0.06) ceramics were prepared by solid-state synthesis process. Their dielectric, thermal and Raman properties were studied. X-ray diffraction analysis shows that the obtained samples possess the perovskite structure with rhombohedral symmetry. SEM results confirm that the ceramics are well sintered and exhibit relative densities higher than 97%. Dielectric measurements revealed that electric permittivity increases, the maximum is broadened and shifted to lower temperature, and local anomaly shows relaxor behavior after Sr doping of NBT. The transition temperature observed by means of differential scanning calorimetry measurements is in good agreement with that obtained from dielectric study. The Raman spectra are similar for all samples in agreement with the X-ray data. The possible origin of the observed effects was discussed.

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POSTER - 51

PHYSICAL PROPERTIES OF NANOSIZED $Ba_{1-x}Ca_xTiO_3$ SOLID-SOLID SOLUTION OBTAINED BY MECHANOCHEMICAL SYNTHESIS

I. Szafraniak-Wiza[1], A. Włódarkiewicz[1] and L. Kozielski[2]
[1]*Institute of Materials Science and Engineering, Poznań University of Technology, Jana Pawła II 24, 61-148 Poznań, Poland*
[2]*Department of Materials Science, University of Silesia, Zytnia 12, 41-200 Sosnowiec, Poland*
izabela.szafraniak-wiza@put.poznan.pl

The barium titanate ($BaTiO_3$) is one of the best-known ferroelectric materials. The substitution of Ba by Ca in the $BaTiO_3$ results in an improvement of the stability of the piezoelectric properties. Recently the barium calcium titanate ($Ba_{1-x}Ca_xTiO_3$) solid solution has attracted great attention because of its applications in the laser systems, electro-optic material for various photorefractive and holographic applications.

We used the mechanochemical method to obtain nanopowder of several solid-solid solutions of $Ba_{1-x}Ca_xTiO_3$ ($0.2 \leq x \leq 0.3$). The main advantage of this method is the room temperature process (which does not need any further temperature treatment) and simple oxide used for synthesis. $Ba_{1-x}Ca_xTiO_3$ was synthesized by high-energy milling in SPEX 8000 Mixer Mill from high purity BaO, CaO and TiO_2 in stoichiometric ratio. The development of the synthesis was controlled by X-ray diffraction. Directly after milling nanopowder exhibits the perovskite structure and the reaction has been completed after 70 h milling.

The properties of pressed nanopowders were investigated by dielectric spectroscopy. The complex dielectric permittivity was studied in temperature range (300 - 500 K) and frequencies (10 Hz - 1 MHz). It is interesting to see that there was no frequency dispersion observed in the measured frequency range for the obtained samples.

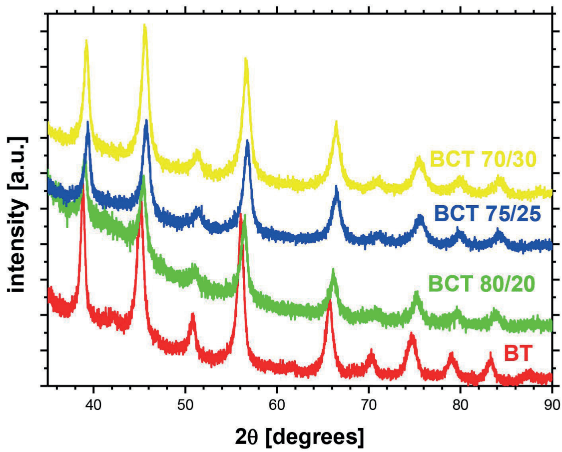

Fig. 1. XRD patterns of $BaTiO_3$ and different $Ba_{1-x}Ca_xTiO_3$ composition obtained after milling for 70 h.

POSTER - 52

PREPARATION AND PROPERTIES OF Bi_3TiNbO_3 OBTAINED BY CONVENTIONAL SOLID STATE REACTION AND MECHANOCHEMICAL SYNTHESIS

I. Szafraniak-Wiza[1] and M. Adamczyk-Habrajska[2]
[1]*Institute of Materials Science and Engineering, Poznań University of Technology, Jana Pawła II 24, 61-148 Poznań, Poland*
[2]*Institute of Technology and Mechatronics, University of Silesia, Zytnia 12, 41-200 Sosnowiec, Poland*
izabela.szafraniak-wiza@put.poznan.pl

Technological interest in of Bi_3TiNbO_9 has arrived due to its ferroelectric and piezoelectric properties that are present up to one of the highest ferroelectric-paraelectric phase transition. Bi_3TiNbO_9 belongs to the family of Aurivillius compounds, generally formulated $[Bi_2O_2][A_{n-1}B_nO_{3n+1}]$, are built up by the intergrowth of Bi-O and pseudo-perovskite layers. Usually Bi_3TiNbO_9 ceramics is prepared by conventional solid state sintering process. From scientific and technological points of view it is important how the mechanochemical treatment affects microstructure, crystal structure as well as the dielectric properties of final ceramic materials. The main advantage of mechanochemical method is room temperature process (which does not need any further temperature treatment), simple oxides used for synthesis and final product consists of nanosized grains that usually results in high density ceramics. The development of the synthesis was controlled by X-ray diffraction and directly after milling nanopowder exhibits the perovskite structure.

The poster will presented details of used method as well as the comparison of microstructure and crystal structure of obtained samples. Authors would like to discuss the results of dielectric spectroscopy investigations, which were carried out temperature range (300 - 1200 K) and frequencies (100 Hz - 1 MHz).

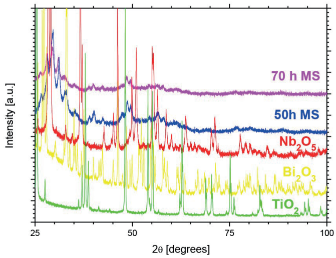

Fig. 1. XRD patterns of Bi_3TiNbO_9 obtained after different milling periods.

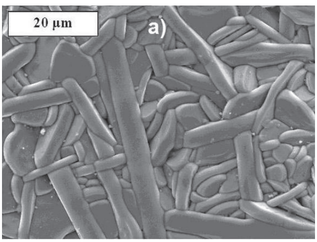

Fig. 2. Scanning electron microscope image of the fracture surface of Bi_3TiNbO_9 obtained by conventional solid state sintering process.

POSTER - 53

ELECTRICAL PROPERTIES OF EPOXY-GLUE / $BiMnO_3$ COMPOSITE

A. Szeremeta[1], A. Molak[1], S. Pawlus[2], J. Koperski[1] and A. Leonarska[1]
[1]Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland
[2]Institute of Physics, University of Silesia (Śląskie Międzyuczelniane Centrum Edukacji i Badań Interdyscyplinarnych), ul. 75 Pułku Piechoty 1A, 41-500 Chorzów, Poland
annaszeremeta90@gmail.com

The electrical properties of composite of two components, epoxy-glue and $BiMnO_3$ ceramics, containing 66 wt% $BiMnO_3$, were studied. Reference samples were $BiMnO_3$ ceramics with sillenite structure [1] and epoxy-glue. Secondary electron images and backscattered electron images were collected for the epoxy and the epoxy-$BiMnO_3$ samples. Scanning electron microscopy showed homogenously distributed $BiMnO_3$ powder in the epoxy matrix. It has been detected that the Bi:Mn ratio was different from the nominal value. Moreover, structure of the samples was determined with use of the XRD measurement in 300 - 450 K range. The electric impedance was measured for frequencies f = 40 Hz - 1 MHz in the 180 - 440 K range. It was analysed with use of electric permittivity ε*(T,f) and modulus M''(T,f) representations. The tested epoxy-$BiMnO_3$ sample exhibited low dielectric losses. The samples of epoxy-$BiMnO_3$ composite show several electric conductivity relaxations. The dominating one is related to activation energy E_a = 0.6 - 1.0 eV, varying with temperature range. Therefore the Vogel-Fulcher-Tammann relationship was applied for relaxation times obtained from M''(T,f) representation. The other processes were not resolved clearly. The relaxation times were discussed in framework of the polymer-ceramic particle interfacial layer model [2].

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POSTER - 54

PHASE TRANSITION IN TRIGLYCINE SULPHATE UNDER DYNAMIC STIMULATION

M. Trybus and B. Woś
Institute of Mathematics and Applied Physics, Rzeszów Technical University, Poland
m_trybus@prz.edu.pl

In the paper we investigate the pyroelectric properties of triglycine sulfate (TGS) samples using fast temperature pulses in both ferroelectric and paraelectric phases. Our previous experiments proved some kind of order in the paraelectric phase, which resulted in pyroelectric response to the fast temperature pulses, above the critical temperature [1]. Many authors investigate phase transition and structural changes of TGS and its doped crystals with use of various methods [2,3]. The aim of this investigations is to find structural origin of ferroelectricity and explain the mechanism of phase transition in TGS family. In our works we use software and hardware solutions designed and constructed by our team. Results of our experiments seem to confirm observations of the "evolution" of local order despite of expected order/disorder character of the phase transition in TGS.

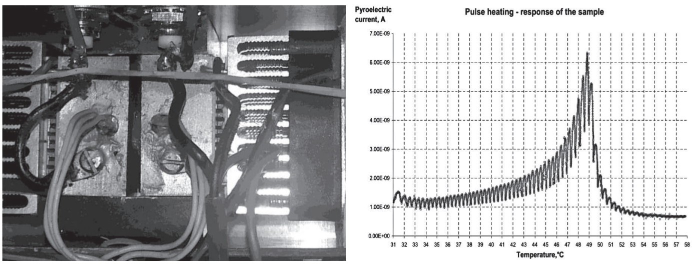

Fig. 1. Sample holder for dynamic measurements (A), pyroelectric response of TGS sample on pulse temperature waveform (B).

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POSTER - 55

ISOMORPHOUS STRUCTURAL PHASE TRANSITION AND PROPERTIES OF NEW DIISOBUTYLAMINE-BASED MOLECULAR-IONIC SALT

M. Wojciechowska[1], P. Szklarz[1], J. Baran[2], W. Medycki[3], A. Piecha-Bisiorek[1] and R. Jakubas[1]

[1]*Faculty of Chemistry, University of Wrocław, Joliot-Curie 14, 50-383 Wrocław, Poland*

[2]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-950 Wrocław 2, PO Box 937, Poland*

[3]*Institute of Molecular Physics, PAS, M. Smoluchowskiego 17, 60-179 Poznań Poland*

martyna.wojciechowska@chem.uni.wroc.pl

The results of systematic structural investigations of haloantimonate(III) and halobismuthate(III) compounds reveal a great variety of different anionic forms. Most of the compounds, described by a general formula $R_aM_bX_{3b+a}$ (where R denotes organic cations, M stands Sb or Bi and X = Cl, Br, I), have a tendency to constitute bi- or polynuclear anions in the crystalline state, where the basic MX6 octahedra share either corners, edges or faces. In spite of the fact that haloantimonates(III) and halobismuthates(III) are characterized by a rich diversity of the anionic networks in the crystal lattices, the ferroelectric properties are limited only to several chemical stoichiometrics namely: $R_5M_2X_{11}$, $R_3M_2X_9$, R_2MX_5 and RMX_4 [1], where the cations are usually small in size alkylammonium ones or five and six-membered heteroaromatic rings. In general, most of the paraelectric-ferroelectric phase transitions are characterized by an 'order-disorder' mechanism connected with the dynamics of the organic counterions.

In search for new acentric and switchable dielectric phase transition (PT) materials we have extended our studies to derivatives containing in the inorganic network bulky second order aliphatic amines. It should be emphasized that simple (1:1) ionic salts built up of expanded second order aliphatic amines, for example diisopropylammonium chloride and diisopropylammonium bromide [2-3] are very promising room temperature ferroelectric materials with the spontaneous polarization comparable with those of well known perovskite-like ferroelectrics ($BaTiO_3$).

In this poster, we present new details of physicochemical properties of organic-inorganic hybrid material, bis(diisobutylammonium) octabromodiantimonate(III) which was found to undergo isomorphous structural phase transition of the first order at 222 K (cooling). The proposed mechanism of the PT was based on the thermal, vibrational (IR) and dielectric studies, while the molecular motions of diisobutylammonium cations were studied by means of proton magnetic resonance (^{1}H NMR). Subsequently, the mechanism of the phase transition is discussed.

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POSTER - 56

PHASE TRANSFORMATIONS OF $KSc(WO_4)_2$: DOMAIN STRUCTURE AND X-RAY STUDIES

M.B. Zapart[1], W. Zapart[1], R. Kowalczyk[1], A. Gagor[2] and M. Maczka[2]
[1]*Institute of Physics, Technical University of Czestochowa, 42-200 Czestochowa, Poland*
[2]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, 50-422 Wroclaw, Poland*
zapart@wip.pcz.pl

The layered compounds $AB(XO_4)_2$, where A is an alkaline ion, B a transition metal ion and X is Mo or W ion, have been extensively studied in the last years. The main interest in these materials is that they have a two-dimensional layered structure [1] and exhibit several structural phase transitions [2]. One of members of this family is $KSc(WO_4)_2$. At T_1 = 309 K the crystal undergoes a structural phase transformation of the second order from a trigonal to a monoclinic phase with a doubling of the unit cell along the three-fold axis of the crystal [2,3]. The second phase transition at T_2 = 288 K was revealed in the EPR experiment [3] and was confirmed by heat capacity measurements [4].
The aim of this contribution is to establish the crystal structure of $KSc(WO_4)_2$ in the para- and ferroelastic phases and to present a more complete description of ferroelastic domain structure and changes in the optical properties of the $KSc(WO_4)_2$ crystal. Also the AFM examination of the structure of the surface layer of a ferroelastic $KSc(WO_4)_2$ crystal is described, and the results obtained are connected with the domain structure observed via microscopy in the polarized light.

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POSTER - 57

OPTICAL STUDIES OF THE FERROELASTIC PHASE TRANSITIONS IN $KFe(MoO_4)_2$

W. Zapart and M.B. Zapart
Institute of Physics, Technical University of Czestochowa, 42-200 Czestochowa, Poland
wzapart@wip.pcz.pl

$KFe(MoO_4)_2$ is a member of trigonal double molybdates and tungstates family (TDM/T) with a general formula $AB(XO_4)_2$ (A=K,Na,Cs,Rb; B=Sc,In,Al,Fe; X=Mo, W). In the high-temperature phase this crystal is trigonal with space group $P\overline{3}m1$[1]. At a temperature of 311 K $KFe(MoO_4)_2$ undergoes a second-order structural phase transition ($\overline{3}mF2/m$) from the trigonal to the monoclinic phase [2]. Another structural phase transition has been found in this crystal at $T_2 = 139$ K [3]; in both low temperature phases a ferroelastic domain structure based on the domain walls W and W' has been established [4].
The contribution deals with the temperature investigations of the morphic birefringence and domain structure evolution in $KFe(MoO_4)_2$. It has been found that the transition at T_2 consists of two transitions separated by the temperature interval of about 0.4 K. Both these transitions are of the first order and are evidenced through a phase front passing, without the domain structure rebuilding. When lowering the temperature a morphic birefringence has been found to decrease in a step way in these transitions. From temperature studies of the morphic birefringence a critical exponent of the order parameter has been estimated.

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POSTER - 58

INFRARED SPECTROSCOPY OF STRAINED $BaTiO_3/SrTiO_3$ SUPERLATTICES ON $DyScO_3$ SUBSTRATES

V. Železný[1], A. Soukiassian[2], X.X. Xi[3] and D.G. Schlom[2]

[1] *Institute of Physics, ASCR, Na Slovance 2, 182 21 Prague 8, Czech Republic*

[2] *Department of Materials Science and Engineering, Cornell University, Ithaca, New York, 14853-1501, USA*

[3] *Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA*

zelezny@fzu.cz

Ferroelectric superlattices of $[(BaTiO_3)_8/(SrTiO_3)_4]_{50}$ grown on the (100) cut of $DyScO_3$, substrates by reactive molecular epitaxy were studied by infrared spectroscopy in a broad temperature range from 8 to 650 K. The polarized spectra were measured along and perpendicular to the c-axis from 30 to 650 cm^{-1}. Simultaneously, the reflectance of the bare substrates was taken under the same conditions to determine their infrared properties. Using the standard technique of effective medium approximation for multilayers systems, we could successfully simulate the far-infrared reflectance of the structures and in this way extract the phonon parameters and determine the superlattice dielectric function.

The superlattice dielectric function shows typical perovskite features with three infrared active phonons. As the superlattice consists of two components, two phonons show two-mode behavior and one one-mode behavior. The most significant feature in spectrum is a peak at 100 cm^{-1}, which begins to appear below 500 K. It corresponds to the polar phonon lowest frequency in perovskite structures and in bulk materials it is considered as a soft mode [1]. In our case, practically no softening is observed and the phonon frequency keeps approximately the same value and only its intensity increases on cooling. The appearance of the peak coincides with the increase of out-of-plane lattice parameter measured by x-ray diffraction. This is interpreted as the appearance of a highly c-axis oriented tetragonal phase. Using infrared spectroscopy we can identify the ferroelectric phase transition into tetragonal phase, which is shifted by 100 K higher in temperature regarding to bulk $BaTiO_3$. On the other hand T_C is lower than that found by Raman scattering for the same superlattices grown on $SrTiO_3$ substrates [2].

When the entire contribution of all polar phonons to static permittivity is summed we obtain the value varying from 200 at 650 K to 450 at 8 K, which is about one half of the value measured in the microwave frequency region [3]. It means there are other low-frequency contributions to permittivity.

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