

## DF 3 Poster Session

Time: Monday 09:30–17:00

Room: P1

DF 3.1 Mon 09:30 P1

**Domain structures, grain boundaries and PTCR effect of ferroelectric barium titanate ceramics** — ●MICHAEL ROESSEL, MIHAIL DAN CROITORU, DAVID MOSER, and OLIVER EIBL — Institut fuer Angewandte Physik, Eberhard Karls Universitaet Tuebingen, Auf der Morgenstelle 10, D-72076 Tuebingen, Germany

Perovskite materials such as barium titanate have many applications as electronic devices. During the cubic to tetragonal phase transition at T<sub>c</sub> (393K) BaTiO<sub>3</sub> exhibits a strong non-linear change of the electrical resistivity (PTCR effect) caused by grain boundaries. The PTCR effect appears in semiconducting barium titanate and is determined by the microstructure of the material. The Heywang model explains the PTCR jump by the existence of a Schottky barrier at the grain boundaries. This model assumes 180° domains, compensating space charges at the grain boundaries. Our TEM studies by diffraction contrast under two-beam and many beam diffraction conditions show irregularly arranged 90° domains. For the analysis of the grain boundaries we concentrate on grains that are close to a pseudocubic [100] orientation. So far 180° domains were not observed experimentally. Compressive stresses in curved sections of the grain boundaries yield a sub-μm domain structure. The appearance of such domain structures might be explained by compensating mechanical stresses during the cubic to tetragonal phase transition. Therefore, Heywangs model is an oversimplification and does not contain a realistic structural model for explaining the electrical resistivity of barium titanate. The goal of our work is a better understanding of the PTCR effect based on an improved grain boundary structure model.

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**Thickness dependent dielectric properties of epitaxial Ba<sub>0.7</sub>Sr<sub>0.3</sub>TiO<sub>3</sub> thin film capacitors** — ●REGINA DITTMANN<sup>1</sup>, RAFAEL PLONKA<sup>2</sup>, NIKOLAY PERTSEV<sup>1</sup>, and RAINER WASER<sup>1,2</sup> — <sup>1</sup>Institut für Festkörperforschung and Center of Nanoelectronic Systems for Information Technology, Forschungszentrum Jülich, 52425 Jülich — <sup>2</sup>Institut für Werkstoffe der Elektrotechnik, RWTH Aachen University of Technology, 52056 Aachen

Single-crystalline all-perovskite SrRuO<sub>3</sub>/Ba<sub>0.7</sub>Sr<sub>0.3</sub>TiO<sub>3</sub> (BST)/SrRuO<sub>3</sub> heterostructures have been grown epitaxially on SrTiO<sub>3</sub> by pulsed laser deposition. The samples exhibit a sharp paraelectric-to-ferroelectric phase transition with a maximum permittivity of about 6660. This value is comparable to that of bulk ceramics and exceeds by several times the highest values reported for BST thin film capacitors. At room temperature, the weak decrease of the permittivity with the BST thickness decreasing from 200 to 10 nm can be explained solely by the thickness-dependent strain relaxation in epitaxial films without assuming the presence of low-permittivity layers at the film/electrode interfaces. Furthermore, the ferroelectric-to-paraelectric phase transition temperature shifts to lower temperatures with decreasing film thickness. As a result, in the low temperature regime, where all samples are in the ferroelectric state, the permittivity increases with decreasing film thickness. This effect is analyzed with the aid of a thermodynamic theory and can be attributed to the influence of the depolarizing field originating from the incomplete screening of the SRO electrodes.

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**Ferroelectric Polarization as the Gradient of Phase Shift in Electron Holography at Atomic Resolution** — ●CHRISTOPHER MATZECK, HANNES LICHTHE, and MARIANNE REIBOLD — Dresden University, Inst. of Structure Physics, Zellescher Weg 16, 01069 Dresden, Germany

The transferred electron wave in Transmission Electron Microscopy is strongly influenced in phase by ferroelectric specimen. This gradient of the phase shift is directly proportional to the projected electric polarization within the sample [1]. Since Electron Holography allows measuring the phase modulation of an object wave, it is also capable of deducing the projected polarization in principle. Discovering ferroelectric dipoles in the phase images of Barium Titanate by means of Electron Holography [2] has opened quantitative characterization of single dipoles and nanodomains directly from phase images. The gradient can be determined numerically by the calculation of the differential quotient of the image data and displayed as a vector plot. This technique shows ferroelectric nanodomains in the range of only a few unit cells.

References:

- [1] H. Lichte, M. Reibold, K. Vogel, M. Lehmann, Ultramicroscopy 93 (2002) 1999
- [2] H. Lichte, M. Reibold, K. Vogel, M. Lehmann, D. Geiger, R. Goldberg, Proc. EMC 2004 (Vol. II), Antwerp, Belgium, 491-492
- [3] The financial support from the Deutsche Forschungsgemeinschaft for the Research Group on Ferroic Functional Components FOR520 is gratefully acknowledged

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**Computer simulation of nanoporous dielectrics** — ●ANTJE ELSNER<sup>1,2</sup>, HELMUT HERMANN<sup>1</sup>, and DIETRICH STOYAN<sup>2</sup> — <sup>1</sup>Institute for Solid State and Materials Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — <sup>2</sup>Institute of Stochastics, Freiberg University of Mining and Technology, D-09596 Freiberg, Germany

New dielectric materials for future semiconducting circuits are needed to compensate the increasing capacity due to decreasing dimensions of interconnects. One promising way to get dielectrics with very low k-values is to use nanoporous material. Porous dielectric materials are simulated by dense random packings assuming a nearly spherical shape of pores. The pores are approximated by spheres whereas the material is represented by the space around. By extending the algorithm to arbitrary continuous diameter distributions it is possible to optimise such structures with respect to maximum porosity and adequate mechanical stability. Basic parameters of the material can be calculated, such as elastic constants and estimations of k-value. Some parameters of the simulated sphere packings can be used to characterize porous media, for example contact number, local density, specific surface area and diameter distribution.

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**Theoretical investigation of fullerene-based ultralow-k dielectrics** — ●YUEKUI WANG<sup>1</sup>, GOTTHARD SEIFERT<sup>1</sup>, and HELMUT HERMANN<sup>2</sup> — <sup>1</sup>TU Dresden, Institute for Physical Chemistry and Electrochemistry, Bergstr. 66b, D-01062 Dresden — <sup>2</sup>IFW Dresden, P.O.Box 27 01 16, D-01171 Dresden

It is one of the urgent problems in microelectronics to develop insulating materials with dielectric constants of less than 2 for future application in semiconducting circuits. Networks of fullerenes connected by bridge molecules are a new class of hypothetical insulating materials with very low static dielectric constant k. It is shown that it is possible to design such materials with k-values of about 1.5. The results are obtained combining total energy and structure optimization calculations.

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**Thickness dependence of specific dc-conductivity of thin-film-ion-conductors** — ●M. SH. ABOUZARI, FRANK BERKEMEIER, TOBIAS STOCKHOFF, and GUIDO SCHMITZ — Westfälische Wilhelms-Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str.10, 48149 Münster

Ion-conducting, amorphous thin films with a thickness of 50-1000 nm are prepared by ion beam sputtering using a glass target of composition 0.2 Li<sub>2</sub>O 0.8 B<sub>2</sub>O<sub>3</sub>. The glass layers are deposited on a silicon substrate between two sputtered electrodes of an Al-Li alloy. Temperature-dependent impedance spectroscopy allows determining the specific dc-conductivities. Recent research work has concentrated on the dependence of the conductivities on the thickness of the films. The conductivity increases significantly with decreasing of film thickness. Close to room temperature, the conductivity of 50 nm thick films exceeds that of 1000 nm thick films by at least one order of magnitude.

DF 3.7 Mon 09:30 P1

**DFT investigation of stepped titanate surfaces** — ●WALTER ALSHEIMER, SIBYLLE GEMMING, and GOTTHARD SEIFERT — Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden.

The structural and electronic properties of vicinal (10n) surfaces of barium titanate were investigated by density-functional band-structure calculations. A plane-wave pseudopotential technique was employed for the (10n) surfaces with n < 5, and systems with larger terraces were studied with a density-functional-based tight-binding method. For the small system sizes, both methods yield considerable structure changes

compared with the bulk geometry. These changes are mostly confined to the step edge and the two unit cells adjacent to it, thus from  $n=4$  on the interaction between two adjacent step edges decreases. The density of electronic states exhibits only minor changes due to the deviations from the nominal stoichiometry at the step. The electric field far above the surface follows the nominal (10n) termination plane. Close to the step edge stronger local variations of the field occur, which may influence the adsorption geometry of polar or polarisable molecules.

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**Ferroelectric properties of Langmuir-Blodgett PVDF-Copolymer films** — ●RAPHAEL TADROS-MORGANE and HERBERT KLIEM — Institute of Electrical Engineering Physics, Saarland University, D66123 Saarbruecken Campus, Germany

Langmuir-Blodgett films are designed as a stack of mono-molecular layers piled up sequentially onto a solid substrate. These layers are transferred from surface active agents trapped at the interface between two dissimilar phases, either liquid-liquid or liquid-gas [1]. However, the P(VDF-TrFE) copolymer is not well suited to this technique. Nevertheless, it is possible to realize ferroelectric thin films using this method. To reach this goal, transfers on a glass substrate were realized for a surface pressure of the interface ranging from 0.5 mN/mm to 5 mN/mm and for concentrations of the copolymer from 0.1 g/l to 0.0001 g/l. For a given number of transfers, here 30, the optimal pressure is about 3mN/mm with a concentration of 0.01 g/l. These samples show true ferroelectric properties like hysteresis loops and switching of the polarization. Films of P(VDF-TrFE) with thicknesses ranging from 2.7 nm to 64 nm prepared by a Langmuir-Blodgett technique at the Institute of Crystallography in Moscow, were electrically characterized. It is found that the coercive fields increase with decreasing sample thickness following a power law. The switching of the polarization yields stretched exponential functions with time constants  $t$  dependent on thickness and temperature.  $t$  increases with decreasing thickness and is thermally activated [2]. Also the initial polarization curves obtained from the unpolarized state are thickness and temperature dependent.

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**Optimization of sol-gel preparation and physical properties of multiferroic  $BiFeO_3$  thin films** — ●SALAH HABOUTI, CLAUS-HENNING SOLTERBECK, SHIVA KUMAR RUDRA, and MOHAMMED ES-SOUNI — Institute for Materials and Surface Technology, University of Applied Sciences, Kiel, Germany

Compared to other deposition techniques, chemical solution deposited  $BiFeO_3$  thin films show lower polarization values. To overcome this problem and optimize the films, influences of various parameters were investigated, like precursor solutions, annealing, temperatures and times, atmosphere etc. Their influence on crystallization, grain growth and microstructure were determined by x-ray diffractometry ( $\theta - 2\theta$ , grazing incidence), electron microscopy, and atomic force microscopy. The effects on the physical properties were investigated by macroscopical measurements of polarization, hysteresis, leakage current, impedance, and piezoelectric activity. Microstructural effects on local electrical properties were studied by means of electrical force microscopy. As a first success the dielectric strength was increased by a factor of 8.

Magnetic properties were measured by a vibrating sample magnetometer and by a scanning magneto-optical Kerr-effect device.

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**Interfacial properties of  $Pb(Zr_{0.52}Ti_{0.48})O_3$  on  $Pt(111)/Ti/SiO_2/Si$  heterostructure** — ●SHIVA KUMAR RUDRA<sup>1</sup>, SALAH HABOUTI<sup>1</sup>, CLAUS-HENNING SOLTERBECK<sup>1</sup>, MOHAMMED ES-SOUNI<sup>1</sup>, VLADIMIR ZAPOROJCHENKO<sup>2</sup>, MICHAEL SCHARNBERG<sup>2</sup>, and FRANZ FAUPEL<sup>2</sup> — <sup>1</sup>Institute for Materials and Surface Technology, University of Applied Sciences, Kiel, Germany — <sup>2</sup>Technical Faculty, Chair of Multicomponent Materials, Christian-Albrechts-University, Kiel, Germany

$Pb(Zr_{0.52}Ti_{0.48})O_3$  (PZT) thin films were processed by sol-gel method on  $Pt(111)/Ti/SiO_2/Si$  substrate heterostructure. Interfacial composition and structure were investigated by means of X-ray photoelectron spectroscopy (XPS) in combination with depth profiling, and grazing incidence X-ray diffraction (GI-XRD). The surface roughness was measured by AFM. Ellipsometric studies as function of depth profiling are also reported. Various annealing temperatures such as 700°C, 650°C and 600°C were considered. Deposited thin films were single layered PZT with 10% Pb excess of the precursor solution. It is shown that with increasing sputtering time the refractive index increases. XPS results show

that prior to sputtering there is an enrichment of Pb on the surface as well as higher Zr/(Zr+Ti) ratio in comparison to nominal composition. The AFM studies show no difference between the as processed and sputtered samples. XPS and XRD results point to the formation of a  $Pt_3Ti$  intermetallic layer at the PZT/Substrate interface.

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**CONDUCTIVITY OF NANOSTRUCTURED MESOPOROUS MCM-41 MOLECULAR SIEVE MATERIALS** — ●MARTYNAS KINKA, JURAS BANYS, JAN MACUTKEVIC, and AGNIUS MESKAUSKAS — Faculty of Physics, Vilnius University, Sauletekio 9, 2040 Vilnius, Lithuania

Dielectric response of water confined in MCM-41 molecular sieve materials showed a power law dispersion, which was assigned to ac conductivity. This process, which occurs at temperatures close to room temperature, was found in all our investigated samples with the pore diameters ranging from 2.0 nm to 3.7 nm. Obtained values of the imaginary part of the complex dielectric permittivity were much larger than that of the bulk water. Such a phenomenon can be explained by the electrical response characteristic of the microstructural electrical network formed by water and hosting mesoporous silica material. The real part of conductivity has been calculated, and the influence of the pores size to electric conductivity and its mechanisms is discussed.

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**Phase and microstructure evolution during  $BaTiO_3$  formation by solid state reactions on rutile single crystals** — ●ANDRIY LOTNYK, STEPHAN SENZ, and DIETRICH HESSE — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

During the synthesis of  $BaTiO_3$  ceramics out of a stoichiometric  $BaCO_3$ - $TiO_2$  mixture the evolution of different intermediate phases can generally be observed. These intermediate products are  $Ba_2TiO_4$  and Ti-rich phases. Using micro chemically designed core shell powders the sequence of forming phases changes. To understand this behavior model experiments are performed using rutile ( $TiO_2$ ) single crystals. The solid state reactions of  $TiO_2$  with  $BaCO_3$  (solid and vapour, respectively) are studied. A  $BaCO_3$  target was electron beam evaporated in a high vacuum system with  $P_{O_2}=1 \times 10^{-2}$  Pa. The substrates were heated in a tube furnace at  $T=300$ - $500^\circ C$  during deposition, followed by a solid-solid reaction at  $575$ - $1100^\circ C$  in vacuum or in air; for the gas-solid reaction, the substrates were heated at  $T=575$ - $1100^\circ C$  directly during deposition. The reaction products were investigated by XRD and TEM. The solid-solid reaction at  $600^\circ C$  for 30 min under vacuum produced the metastable intermediate  $Ba_2TiO_4$  phase while the reaction in air resulted in the formation of  $BaTiO_3$ . Well-oriented products are formed on (110), (100), (101)  $TiO_2$  and polycrystalline phases were identified on (001)  $TiO_2$ .

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**Investigation of Li diffusion in spinel-type structured  $Li_4Ti_5O_{12}$  by means of solid state NMR and impedance spectroscopy** — ●M. WILKENING, W. IWANIAK, R. AMADE, and P. HEITJANS — Hannover University, Institute of Physical Chemistry and Electrochemistry, D-30167 Hannover

The cubic spinel oxides  $Li_{1+x}Ti_{2-x}O_4$  ( $0 \leq x \leq \frac{1}{3}$ , space group  $Fd3m$ ) are promising anode materials for lithium-ion rechargeable batteries. The end member of the Li-Ti-O series,  $Li_4Ti_5O_{12}$ , can accommodate Li ions up to the composition  $Li_7Ti_5O_{12}$ . Whereas a number of studies focus on the electrochemical behaviour of Li insertion into and Li diffusion in the Li intercalated material, only few investigations of Li dynamics in the non-intercalated host material  $Li_4Ti_5O_{12}$  are reported so far. Here, the Li diffusion in pure-phase microcrystalline  $Li_4Ti_5O_{12}$  with an average particle size in the  $\mu m$  range was probed by  $^7Li$  solid state NMR spectroscopy using spin-alignment echo (SAE) and spin-lattice relaxation (SLR) measurements. Between  $T = 295$  K and 400 K extremely slow Li jump rates  $1/\tau$  ranging from  $1 s^{-1}$  to  $1000 s^{-1}$  were directly obtained by recording the decay of spin-alignment echoes at a Larmor frequency of 155 MHz as a function of mixing time and constant evolution time.  $1/\tau(1/T)$  follows Arrhenius behaviour with an activation energy  $E_A^{SAE}$  of about 0.85 eV. Interestingly,  $E_A^{SAE}$  is comparable to activation energies deduced from conductivity measurements rather than from SLR-measurements,  $E_A^{SLR} \approx 0.28$  eV.

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**Effect of anion substitution on Li diffusion in  $\text{Li}_x\text{TiS}_{2-y}\text{Se}_y$ : Solid state NMR results** — ●M. WILKENING<sup>1</sup>, S. INDRIS<sup>1</sup>, P. HEITJANS<sup>1</sup>, J. WONTCHEU<sup>2</sup>, W. BENSCH<sup>2</sup>, T. BREDOW<sup>3</sup>, and M. BINNEWIES<sup>4</sup> — <sup>1</sup>Hannover University, Institute of Physical Chemistry and Electrochemistry, D-30167Hannover — <sup>2</sup>University of Kiel, Institute of Inorganic Chemistry, D-24098 Kiel — <sup>3</sup>Hannover University, Theoretical Chemistry, D-30167 Hannover — <sup>4</sup>Hannover University, Institute of Inorganic Chemistry, D-30167Hannover

Li intercalated  $\text{TiS}_2$  is known as a fast two-dimensional ionic conductor. At 298 K the diffusion coefficient  $D_{\text{Li}}$  turns out to be about  $10^{-14} \text{ m}^2\text{s}^{-1}$  and the corresponding Li residence time is of the order of 1  $\mu\text{s}$ . It is of general interest to explore a possible effect of anion substitution on diffusion of small cations. The system  $\text{Li}_x\text{TiS}_{2-y}\text{Se}_y$  is stable over the whole intercalation range ( $0 \leq x \leq 1$ ) and shows a single-phase structure for all compositions. Due to these properties it represents a singularly well-defined series of materials to investigate whether Li diffusion is influenced by the substitution of selenium anions for sulfur anions having nearly the same ionic radii. Li diffusion in  $\text{Li}_x\text{TiS}_{2-y}\text{Se}_y$  was studied by means of <sup>7</sup>Li solid state NMR. First lineshape analyses of data at a Larmor frequency of 78 MHz and temperatures between 140 K and 450 K indicate, that the Li mobility is slower in, e. g.,  $\text{Li}_{0.7}\text{TiS}_2$  than in the pure end member  $\text{Li}_{0.7}\text{TiS}_2$ . Supported by the DFG (SPP 1136).

DF 3.15 Mon 09:30 P1

**Phonon modes of monoclinic  $\text{BiB}_3\text{O}_6$**  — ●TH. MÖLLER<sup>1</sup>, A. GÖSSLING<sup>1</sup>, W.-D. STEIN<sup>1</sup>, P. BECKER<sup>2</sup>, L. BOHATÝ<sup>2</sup>, and M. GRÜNINGER<sup>3</sup> — <sup>1</sup>2nd Physical Institute, University of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — <sup>2</sup>Institute of Crystallography, University of Cologne, Zülpicher Str. 49b, 50674 Cologne, Germany — <sup>3</sup>2nd Physical Institute, RWTH Aachen, Huyskensweg, 52056 Aachen, Germany

The large optical nonlinearities of  $\text{BiB}_3\text{O}_6$ , a polar, non-ferroelectric crystal, open up a rich field of applications for frequency conversion of laser light via  $\chi^{(2)}$  and  $\chi^{(3)}$  processes, e.g. phase-matched second harmonic generation (SHG) or optical parametric oscillation (OPO) and stimulated Raman scattering (SRS). The exceptional optical nonlinearities of  $\text{BiB}_3\text{O}_6$  have been attributed to the hyperpolarisabilities of the  $[\text{BO}_3]$  structural units and the  $[\text{BiO}_6]$  units with a lone electron pair. Lattice dynamics studies are required for a quantitative description of the crystal structure and are the basis for an interpretation of the nonlinear optical interaction. We present a detailed study of the phonon modes of this monoclinic compound based on polarized reflectivity measurements on single crystals. The spectra are analysed by means of a generalized Drude-Lorentz model, which allows us to resolve the modes of A and B symmetry.

DF 3.16 Mon 09:30 P1

**Electronic structure and optical properties of sodium titanium diphosphate crystals** — ●OLEKSANDR OLIYNYK<sup>1</sup>, YURIY HIZHNYI<sup>1</sup>, SERGIY NEDILKO<sup>1</sup>, VOLODYMYR BOJKO<sup>2</sup>, PAVLO NAGORNYI<sup>1</sup>, and MYKOLA SLOBODYANIK<sup>1</sup> — <sup>1</sup>Kyiv National Taras Shevchenko University, 2, block 1, Hlushkova av., 03680, Kyiv, Ukraine — <sup>2</sup>National Agriculture University, Geroiv Oborony st., 03041, Kyiv, Ukraine

Sodium titanium diphosphate crystals  $\text{NaTiP}_2\text{O}_7$  belong to the family of the complex phosphates of the alkaline and polyvalent metals.  $\text{NaTiP}_2\text{O}_7$  can be considered as the base for development of new crystallophosphors. Such new materials can be designed by making the solid state solutions on the base of sodium titanium diphosphate matrixes.

Both experimental and theoretical investigations of  $\text{NaTiP}_2\text{O}_7$  optical properties are carried out. Luminescence spectra are measured in 350 - 850 nm spectral region in temperature range 4.2 - 300 K. Several bands of luminescence in blue-green and orange-red region were found in the spectra. The electronic structure of  $\text{NaTiP}_2\text{O}_7$  is calculated by full potential Linear Augmented Plane Wave (FLAPW) method implemented in WIEN2k program code [1]. The structures of the electronic bands, the energy dependencies of the components of dielectric tensor, reflection and absorption spectra of  $\text{NaTiP}_2\text{O}_7$  are calculated. Results of the calculations are compared with experimental data and with results of the electronic structure calculations of several other complex phosphates. The origin of the  $\text{NaTiP}_2\text{O}_7$  luminescence bands is discussed.

[1] P. Blaha, et. al., 2001, ISBN 3-9501031-1-2

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**Muon spin rotation studies of hydrogen-bonded ferroelectrics and antiferroelectrics** — ●ELVEZIO MORENZONI, HUBERTUS LUETKENS, ANDREAS SUTER, DIMITRY ESHCHENKO, ALEX AMATO, THOMAS PROKSCHA, and ROBERT SCHEUERMANN — Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

We present muon spin rotation and relaxation measurements in hydrogen bonded systems of the KDP family. The positive muon and muonium behave like light proton and hydrogen isotopes and can be used to study stability and defect reactions of positive and neutral hydrogen interstitials in these ferroelectric or antiferroelectric materials, where hydrogen point defects are believed to affect the optical-absorption properties. A substantial fraction of the muons implanted into the crystals appear as neutral interstitial not reacting with the host. The hyperfine structure shows a slight axial anisotropy but is otherwise similar to that of free muonium. In the positively charged state, part of the muons form a hydrogen bond with an oxygen. In the ferroelectric  $\text{KH}_2\text{PO}_4$  as well as in the antiferroelectric  $\text{NH}_4\text{H}_2\text{PO}_4$  we observe spontaneous precession of the muon spin in the nuclear dipolar field of the proton of the O-H bond. The temperature dependence of this frequency exhibits a marked shift at the phase transition. Our results suggest that it is possible to use this and other parameters (such as the width of the local static dipolar field) as a microscopic measure of the order parameter of the phase transition. This is interesting especially for the study of proton and deuteron glasses where the order parameter characterizing the glass transition is not accompanied by a macroscopic field.

DF 3.18 Mon 09:30 P1

**Effect of anion substitution on Li diffusion in  $\text{Li}_x\text{TiS}_{2-y}\text{Se}_y$ : Quantum-chemical calculations** — ●T. BREDOW<sup>1</sup>, M. WILKENING<sup>2</sup>, S. INDRIS<sup>2</sup>, P. HEITJANS<sup>2</sup>, J. WONTCHEU<sup>3</sup>, and W. BENSCH<sup>3</sup> — <sup>1</sup>Hannover University, Theoretical Chemistry, D-30167 Hannover — <sup>2</sup>Hannover University, Institute of Physical Chemistry and Electrochemistry, D-30167 Hannover — <sup>3</sup>University of Kiel, Institute of Inorganic Chemistry, D-24098 Kiel

The Li intercalation of titanium chalcogenides  $\text{TiS}_2$ ,  $\text{TiSe}_2$  and  $\text{TiSe}_2$  is investigated quantum-chemically at density functional level in combination with a crystalline orbital approach based on atom-centered basis functions. Periodic supercells are used to model the  $\text{Li}_x\text{TiS}_{2-y}\text{Se}_y$  system. The electronic structure of the intercalation compounds, the electric field gradients at the Li lattice positions, and the activation barriers for elementary steps of the Li ion migration are calculated and compared to experimental results obtained by NMR spectroscopy. A strong dependence of both electric field gradient and migration barrier on the local environment of the Li ions is observed. The activation energy is similar for  $\text{TiS}_2$  and  $\text{TiSe}_2$  host systems but differs for  $\text{TiSe}_2$ . Supported by the DFG (SPP 1136).

DF 3.19 Mon 09:30 P1

**Fabrication and characterization of the electrical and dielectric properties of thin insulating films for the application in superconducting devices** — ●VEIT GROSSE<sup>1</sup>, RALF BECHSTEIN<sup>1</sup>, ROBERT PIETZCKER<sup>1</sup>, FRANK SCHMIDL<sup>1</sup>, INGO USCHMANN<sup>2</sup>, and PAUL SEIDEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, D-07743 Jena — <sup>2</sup>Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena

Thin dielectric films of strontium titanate (STO) as well as zinc oxide (ZnO) were deposited on  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ -layers on STO-substrates by Pulsed Laser Deposition. In the case of STO, X-Ray investigations showed good crystalline quality and orientation in c-direction due to the good match of the lattice parameter. First results to the epitaxial growth of ZnO will be presented. With regard to the application in superconducting devices the electrical and dielectric properties of these films were investigated on capacitor-like structures. The time of oxygen annealing after deposition and the material of the top electrode (e.g. YBCO, Au) were varied to analyse the influence of these factors on the conduction process. We also investigated the dependence of the dielectric permittivity on temperature in the range from 300 to 4.2 K and on a electric bias field. We compare these results with measurements on amorphous insulating films (e.g.  $\text{SiO}_2$ ,  $\text{CeO}_X$ ) in Au/insulator/Au-systems.

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**Electrical, photoelectrical and optical properties of Ru-doped  $\text{Bi}_{12}\text{M}(\text{Si},\text{Ti})\text{O}_{20}$  crystals** — ●VERA MARINOVA<sup>1</sup>, S. H. LIN<sup>2</sup>, K. Y. HSU<sup>2</sup>, BORIANA MIHAILOVA<sup>1</sup>, and ULRICH BISMAYER<sup>1</sup> — <sup>1</sup>Universität Hamburg, Mineralogisch-Petrographisches Institut, Grindelallee 48, D-20146 Hamburg — <sup>2</sup>Department of Photonics and Institute of Electro-Optical Engineering, National Chiao Tung University, 1001 Ta Hsueh Road, Hsinchu 30050, Taiwan

$\text{Bi}_{12}\text{TiO}_{20}$  (BTO) and  $\text{Bi}_{12}\text{SiO}_{20}$  (BSO) sillenite-type crystals doped with different concentration of ruthenium are grown using the Top Seeded Solution Growth method (TSSG) and by the Czochralski technique, respectively. The addition of ruthenium shifts the optical absorption to the red and to the near IR spectral range for BSO and BTO, respectively. It is found that the relaxation (dark decay) of the light induced absorption consists of fast (transient) and a slow (persistent) component, suggesting participation of shallow levels in a charge-transport mechanism. The dark conductivity follows the Arrhenius law. The Ru-doped BSO crystal shows very fast response time during holographic recording at 633 nm and 647 nm. The Ru-doped BTO possesses infrared sensitivity and photorefractive gratings are successfully recorded at 790 nm and 825 nm.

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**Thermal motion induced resonant \*forbidden\* reflections in Ge and ZnO** — ●ALEXEY ORESHKO<sup>1</sup>, VLADIMIR DMITRIENKO<sup>2</sup>, and ELENA OVCHINNIKOVA<sup>1</sup> — <sup>1</sup>M.V.Lomonosov Moscow State University, Physical Department, Moscow, Russia, 119992 — <sup>2</sup>V.A.Shubnikov Institute of Crystallography RAS, Moscow, Russia, 119333

In this report we discuss thermal-motion-induced (TMI) \*forbidden\* reflections. Atomic displacements can change the symmetry of an atomic site, and thus induce an additional anisotropy of the atomic scattering factor near an absorption edge and therefore give rise to Bragg reflections, otherwise forbidden. Since TMI scattering arises from the relative displacement of adjacent atoms, its strength depends crucially on the thermal population of optical phonons modes. The search for suitable materials in which to study this effect is therefore governed by the requirements for: (1) a suitable space group; (2) site symmetry; (3) an absorption edge resonance at a wave-length suitable for crystal diffraction; (4) a low-lying optical phonon mode; (5) a high quality single crystal sample. Ge, which crystallizes with the diamond structure, and w-ZnO, which crystallizes with the Wurtzite structure, satisfy the above conditions. Strongly temperature dependent TMI reflections were recently observed in Ge and w-ZnO. Owing to interference with the temperature-independent contribution, their intensities can increase and decrease with temperature. In this report we present ab initio simulations of the temperature dependence and diffraction spectra for Ge and w-ZnO.

DF 3.22 Mon 09:30 P1

**Construction of a wavelength filter in Lithiumniobat by irradiation** — ●STEFANIE HAUBRICH, MATZ HAAKS, KONRAD PEITHMANN, and KARL MAIER — Helmholtz-Institut für Strahlen- und Kernphysik der Rheinischen Friedrich-Wilhelms-Universität zu Bonn, Nußallee 14-16, 53115 Bonn

Lithiumniobat ( $\text{LiNbO}_3$ ) is an interesting ferroelectric material well suited for applications in holographic storage and integrated optics. Periodic structures in the refractive index in the propagation direction of the light generate a frequency sensitive filter. Recent experiments proved that the refractive index of  $\text{LiNbO}_3$  can be changed by irradiation with light high energy ions. [1] In a proof of principle we create a periodic pattern of the refractive index by irradiating a  $\text{LiNbO}_3$  crystal with  $^3\text{He}$ . Thereby the ion beam is shaded by a parallel array of thin Tantalum foils arranged with a distance of 3  $\mu\text{m}$ . For an exact positioning of the array a 20 nm layer of Aluminum is deposited on the crystals surface and structured with parallel lines in 3  $\mu\text{m}$  distance by laser ablation. The position can be controlled by interference between both line-structures.

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DF 3.23 Mon 09:30 P1

**Ultrasound Investigations of  $\text{BaTi}_{1-x}\text{Sn}_x\text{O}_3$  Ceramics** — ●ULRICH STRAUBE<sup>1</sup>, LUDWIG GESKE<sup>1</sup>, RALF STEINHAUSEN<sup>1</sup>, HANS THEO LANGHAMMER<sup>1</sup>, HORST BEIGE<sup>1</sup>, and HANS-PETER ABICHT<sup>2</sup> — <sup>1</sup>Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, Friedemann-Bach-Platz 6, D-06108 Halle/Saale (Germany) — <sup>2</sup>Martin-Luther-Universität Halle-Wittenberg, Fachbereich Chemie, Karl-Mothes-Str. 2, D-06120 Halle/Saale (Germany)

$\text{BaTi}_{1-x}\text{Sn}_x\text{O}_3$  (BTS) ceramics can be interpreted as a system with more or less diffuse phase transition behaviour depending on the Sn content of the material. BTS belongs to the class of  $\text{BaTiO}_3$  based environmental-friendly solid solutions, which possesses similar properties like the classical lead-containing relaxors and is becoming an interesting candidate for future applications. Its dielectric and electromechanical resonance properties were already reported in [1]. In the present study the elastic stiffness coefficients were determined by the ultrasound impulse overlap technique at a frequency of 5 MHz allowing the simultaneous determination of sound velocity and attenuation. Elastic properties in a broad temperature range with compositions of  $x \leq 0.15$  were obtained. The cubic-tetragonal and the tetragonal-orthorhombic phase transitions are accompanied by anomalies of the sound velocities and the ultrasound attenuation. Sound velocities show minima whereas attenuation increases strongly especially near the cubic-tetragonal transition. Effects of the acoustic dispersion of the elastic data of BTS are discussed.

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DF 3.24 Mon 09:30 P1

**Growth, structural, electrical and optical properties of complex perovskite-type  $\text{Pb}_{0.78}\text{Ba}_{0.22}\text{Sc}_{0.5}\text{Ta}_{0.5}\text{O}_3$  single crystals** — ●VERA MARINOVA<sup>1</sup>, BORIANA MIHAILOVA<sup>1</sup>, DIMITRINA PETROVA<sup>2</sup>, THOMAS MALCHEREK<sup>1</sup>, and ULRICH BISMAYER<sup>1</sup> — <sup>1</sup>Universität Hamburg, Mineralogisch-Petrographisches Institut, Grindelallee 48, D-20146 Hamburg — <sup>2</sup>South-West University Neofit Rilski, 2700 Blagoevgrad, Bulgaria

$\text{Pb}_{0.78}\text{Ba}_{0.22}\text{Sc}_{0.5}\text{Ta}_{0.5}\text{O}_3$  (PBST) single crystals are prepared by the High Temperature Solution Growth (HTSG) method using a flux solution with composition  $\text{PbO} : \text{PbF}_{0.2} : \text{B}_2\text{O}_3 = 0.75 : 0.23 : 0.2$ . The growth conditions for a solid-state phase synthesis were established. The growing process was performed in platinum crucibles in temperature range 1430-1193 K with cooling velocity of 0.5 deg/h. The obtained crystals are cubic-shaped with approximately 1  $\text{cm}^3$  of size. X-ray diffraction data revealed a doubled perovskite-type structure for this newly synthesized compound. The PBST sample was analysed by electrical, optical, and inelastic light scattering measurements. The phase transition was studied by dielectric measurements in the temperature interval from 77 K to 400 K.

DF 3.25 Mon 09:30 P1

**Temperature evolution of the phonon anomalies in relaxor ferroelectric  $\text{PbSc}_{0.5}(\text{Nb},\text{Ta})_{0.5}\text{O}_3$**  — ●BORIANA MIHAILOVA<sup>1</sup>, ULRICH BISMAYER<sup>1</sup>, BERND GÜTTLER<sup>2</sup>, RAINER STOSCH<sup>2</sup>, and MARIN GOSPODINOV<sup>3</sup> — <sup>1</sup>Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelallee 48, D-20146 Hamburg, Germany — <sup>2</sup>Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — <sup>3</sup>Institute of Solid State Physics - Bulgarian Academy of Sciences, Blvd. Tzarigradsko Chausee 72, 1784 Sofia, Bulgaria

Single crystals of stoichiometric  $\text{PbSc}_{0.5}\text{Ta}_{0.5}\text{O}_3$  (PST) and  $\text{PbSc}_{0.5}\text{Nb}_{0.5}\text{O}_3$  (PSN) as well as mixed  $\text{PbSc}_{0.5}(\text{Nb}_x\text{Ta}_{1-x})_{0.5}\text{O}_3$  compounds are investigated by Raman scattering and X-ray diffraction. The temperature dependence of the polarized Raman spectra reveals different preferred ferroic species in PST and PSN. Near the dielectric constant maximum cooperative shifts of Pb atoms in respect to the oxygen sheets perpendicular to the cubic body diagonal occur in larger spatial regions for PST than for PSN. On cooling down this structural modification becomes preferential for PST, thus giving rise to highly anisotropic ferroelectric domains. In PSN the temperature decrease favours B-cation deviations from the  $\text{BO}_6$ -octahedral centres, which leads to formation of small-sized polar clusters distributed in the isotropic matrix. Near 180 K PST undergoes an additional phase transition, which involves reduction of the rotation symmetry. The loading of Nb into PST affects strongly the nanoscale domain texture and the structural transformations that occur on cooling down.

DF 3.26 Mon 09:30 P1

**Dielectric properties of BT-LMT mixed ceramics** — ●POVILAS KEBURIS<sup>1</sup>, JURAS BANYS<sup>1</sup>, ALGIRDAS BRILINGAS<sup>1</sup>, ANDREI SALAK<sup>2</sup>, and VICTOR M. FERREIRA<sup>3</sup> — <sup>1</sup>Department of Radiophysics, Vilnius University, Lithuania — <sup>2</sup>Department of Ceramics and Glass Engineering/CICECO, University of Aveiro, Portugal — <sup>3</sup>Department of Civil Engineering/CICECO, University of Aveiro, 3810-193 Aveiro, Portugal

Ceramics of  $(1-x)\text{BaTiO}_3-x\text{La}(\text{Mg}_{1/2}\text{Ti}_{1/2})\text{O}_3$  with  $x=0.025$  (0.975BT-0.025LMT) were dielectrically investigated over the extended frequency

range. Dielectric studies have been performed at 20 Hz to 3 GHz within the temperature interval of 100 K - 500 K. Apparent relaxor behaviour was revealed to set in when the BT-type three phase transitions become diffuse and merge at low temperatures. Maximums of both imaginary and real parts of the dielectric permittivity are shifted to lower temperatures comparing to pure BT and in the temperature ranges close to phase transitions show strong frequency-dependent behaviour, typical for relaxors. Dynamics of the phase transitions are discussed.

DF 3.27 Mon 09:30 P1

**Dielectric spectra of PMN-PSN-PZN ceramics** — ●JURAS BANYS<sup>1</sup>, JAN MACUTKEVIC<sup>1</sup>, ALGIRDAS BRILINGAS<sup>1</sup>, JONAS GRIGAS<sup>1</sup>, ANDRIS STERNBERG<sup>2</sup>, VISMANTS ZAULS<sup>2</sup>, and KARLIS BORMANIS<sup>2</sup> — <sup>1</sup>Department of Radiophysics, Faculty of Physics, Vilnius University, Lithuania — <sup>2</sup>Institute of Solid State Physics University of Latvia, Latvia

The dielectric dispersion of various ceramics  $\text{PbSc}_{1/2}\text{Nb}_{1/2}\text{O}_3$ - $\text{PbZn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ - $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$  (PSN-PMN-PZN) was measured in very wide frequency range and analyzed in terms of distributions of relaxations times, using Tichonov regularization method. Symmetric and narrow distribution of relaxation times is obtained at higher temperature. On cooling the distribution function becomes asymmetrically shaped and second maximum appears. The longest relaxation times diverge according to Vogel-Fulcher law, however the most probable relaxation time diverges according to Arrhenius law. Enough high activation energy (0.5-0.2 eV) of most probable relaxation times show that in both parts of distribution of relaxation times dominate strongly correlated relaxation. The freezing of dynamics of polar nano regions in PMN-PSN-PZN ceramics must understood as uninterrupted process on cooling from T\$0\$ to 0 K. Only at very low temperatures (T<50 K) the contribution of polar nano region becomes enough small, so that the contribution of non-polar matrix can be clearly resolved. The obtained activation energy of fluctuations in non-polar matrix is much smaller as activation energy of most probable relaxation times.

DF 3.28 Mon 09:30 P1

**Broadband dielectric spectroscopy of PSN ceramics** — ●ROBERTAS GRIGALAITIS<sup>1</sup>, JURAS BANYS<sup>1</sup>, ALGIRDAS BRILINGAS<sup>1</sup>, ANDRIS STERNBERG<sup>2</sup>, VISMANTS ZAULS<sup>2</sup>, and KARLIS BORMANIS<sup>2</sup> — <sup>1</sup>Faculty of Physics, Vilnius University, 9 Sauletekio str., 10222 Vilnius, Lithuania — <sup>2</sup>Institute of Solid State Physic, University of Latvia, 8 Kengaraga str., 1063 Riga, Latvia

One of relaxor materials is  $\text{PbSc}_{1/2}\text{Nb}_{1/2}\text{O}_3$  (PSN). In this material the spontaneous transition to ferroelectric phase and also the drastical change in dielectric properties due to the ordering of B' and B'' cations was observed [1]. As is known that relaxors exhibit broad frequency dispersion and huge distribution of relaxation times we have studied the dielectric properties of PSN ceramics in the frequency range from 20 Hz to 3 GHz because no data about dielectric permittivity measurements above 1 MHz was found. The obtained results show a high diffusive peak of the dielectric permittivity and behaviour typical to ferroelectric relaxors above 360 K. In order to deal about the dielectric properties and relaxation processes in PSN in more detail we calculated the relaxation time distribution in these ceramics according to the methodology adopted in [2] and compared with PMN relaxation time distribution [3].

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DF 3.29 Mon 09:30 P1

**Metastable polar structures in the uniaxial relaxor  $\text{Sr}_{0.61}\text{Ba}_{0.39}\text{Nb}_2\text{O}_6$ :Ce studied by piezoresponse force microscopy** — ●VLADIMIR V. SHVARTSMAN and WOLFGANG KLEEMANN — Angewandte Physik, Universität Duisburg-Essen, 47048 Duisburg

Strontium-barium titanate  $\text{Sr}_x\text{Ba}_{1-x}\text{Nb}_2\text{O}_6$  (SBN) based materials comprise a special group of relaxor ferroelectrics, which belong to the random-field Ising model (RFIM) universality class [1]. In accordance with the theory of 3D RFIM systems a metastable multidomain state appears on cooling through  $T_c$ , which is expected to relax slowly in time towards the single domain state [2]. We present the results of studies of the polar structures in a SBN single crystal doped with cerium (SBN:Ce) by piezoresponse force microscopy. The appearance of fractal-like nan-

odomains was found on cooling from the paraelectric state. These nanodomains are metastable and grow slowly in the course of time according to a logarithmic law as predicted [2]. At elevated temperatures the decay of the nanodomains takes place, but even above  $T_c$  areas of correlated polarization were observed. We suggest that they correspond to agglomerates of polar nanoregions formed via the ferroelectric mean-field of the system.

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