DF 12: Poster II

Time: Wednesday 9:30–12:30 Location: P5

DF 12.1 Wed 9:30 P5

Cr doping of epitaxial $PbZr_{0.2}Ti_{0.8}O_3$ films — •Ludwig Feigl[1], Eckhard Pippel[1], Ionela Vrejoiu[1], Rüdiger-A. Eichel[2], Emre Erdem[2], Roland Mattheis[3], Marin Alexe[1], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [2]Institut für Physikalische Chemie I, Universität Freiburg, D-79104 Freiburg, Germany — [3]Institut für Photonische Technologien (IPHT), D-07702 Jena, Germany

RBS investigations suggested that Cr impurities are present in epitaxial PZT20/80 films deposited from a stoichiometric $Pb_{1.1}Zr_{0.2}Ti_{0.8}O_3$ target by PLD. To investigate the possible impact of these impurities on the properties of the films, Cr doped PZT20/80 films were deposited onto a $SrRuO_3$ electrode grown on a vicinal (100) $SrTiO_3$ substrate. Various dopant concentrations can be achieved by alternately ablating a pure and a highly doped PZT20/80 target. The structural properties are investigated by means of TEM both in conventional and in high resolution scanning mode combined with EDX. Measurements of the polarization, the dielectric constant and the leakage current in dependence on the applied voltage were performed. The Schottky model is used to derive the electronic properties of the film. The Cr is found to (I) increase the leakage current through a reduction of the Schottky barrier; (II) change the film growth by facilitating relaxation. As shown by EPR, Cr is incorporated at the octahedrally coordinated [Zr,Ti]-site, acting as an acceptor and favoring a directly coordinated oxygen vacancy to the chromium center for partial charge compensation. The dipole is oriented parallel to the spontaneous polarization.

DF 12.2 Wed 9:30 P5

Anomalous strain hysteresis of poled Nd–Mn-doped PZT fibres — •Christoph Pientschke[1], Ralf Steinhausen[1], Horst Beige[1], Reinhard Krüger[2], Tobias Müller[2], Uta Helbig[2], Dieter Sporn[2], Carsten Schuh[3], Stefan Denneler[3], and Hugo Schlich[4] — [1]Martin-Luther-University Halle, Physics Department, PFM, 06099 Halle — [2]Fraunhofer ISC, Würzburg — [3]Siemens AG, CT MM 2, Munich — [4]MaTeck GmbH, Jülich

PZT fibres were produced using the sol–gel process. The PZT was doped with 2 mol% neodymium and 1.1 or 0.75 mol% manganese. After sintering at 900 °C the fibres were fine grained (grain size $\approx 1\mu$m). The fibres were embedded in a polymer for characterisation. The resulting 1–3-composites were poled with a DC voltage for $1\frac{1}{2}$ hours. By applying a bipolar sinusoidal voltage with high amplitude (7 kV/mm) and a frequency of 10 Hz the strain and polarisation were measured. The resulting strain-loops are strongly asymmetric. For the half period with applied fields parallel to the poling field the strain loop exhibits a rather linear shape. For the half period in reversed direction the loop inflates and closes with hardly no strain change. The asymmetry of strain-loops is more pronounced for smaller grains. For samples with 1.1 mol% Mn strain switching seems to be suppressed between room temperature up to 80 °C. The asymmetry of the strain loops is switchable by a subsequent poling process. The blocking of strain switching was proved by measurements of the piezoelectric coefficient d_{33} with superimposed electric field. For 0.75 mol% Mn-content strain switching occurs. All these properties are believed to be a feature of the ceramics.

DF 12.3 Wed 9:30 P5

Local ferroelectric and magnetic measurements on multiferroic $BiCrO_3$ thin films — •Denny Köhler[1], Ulrich Zerweck-Trogisch[1], Christian Loppacher[3], Stephan Geprägs[2], Sebastian T. B. Gönnenwein[2], Rudolf Gross[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, München — [3]Laboratoire de Matériaux et Microélectronique de Provence, Universités Paul Cézanne, Marsaille

We present low-temperature noncontact-AFM investigations in combination with Kelvin Probe Force Microscopy (KPFM) and Magnetic Force Microscopy (MFM) to study the magnetic properties of $BiCrO_3$ thin films on the nm length scale. In addition, we investigated the ferroelectric properties of $BiCrO_3$ thin films by Piezoresponse Force Microscopy (PFM) and compared them to macroscopic hysteresis measurements. The samples have been prepared as described in [1].

The ferroelectric characteristics were measured both above and below the magnetic and ferroelectric phase transition temperatures of $BiCrO_3$. We compare the local PFM measurements with the global properties of the $BiCrO_3$ films obtained from polarization versus applied electric field curves both at room and low temperature.

[1] S. Geprägs et al., *Phil. Mag. Lett.* **87**: 141-147 (2007)

DF 12.4 Wed 9:30 P5

Visualization of elastic properties by use of the slowness surface — •Leonore Wiehl and Eiken Haussühl — Institut für Geowissenschaften, Goethe-Universität Frankfurt, D-60438 Frankfurt

The elastic properties of crystals are described by a tensor of forth rank, which may have up to 21 different components, depending on symmetry. In general the inspection at a first glance of just these coefficients gives no detailed idea, how elasticity varies with crystal direction. Therefore representation surfaces are used for visualization, which help to correlate elastic properties with other physical properties and with the crystal structure. For this purpose most often the longitudinal elastic stiffness is plotted, which represents the elastic "hardness"of a crystal in direction of the applied pressure. More detailed information, though seldom used, provides the refraction surface, or slowness surface [1]. It represents the reciprocal phase velocities of elastic waves. The slowness surface is a surface of 6th degree in the velocities and consists of three separate sheets corresponding to the three elastic waves which propagate in each wave normal direction (one quasi-longitudinal and two quasi-transverse). A program was written, which calculates from the measured elastic coefficients of a crystal with arbitrary symmetry the wave velocities and polarization vectors for a given wave normal by solving the Christoffel equation and plots sections through the slowness surface in any desired orientation. As an example, the elastic properties of $(C_5H_{11}NO_2)_2(CuCl_2)_3{\cdot}2H_2O$ are discussed.

[1] F. I. Fedorov: Theory of Elastic Waves in Crystals. Plenum Press, New York, 1968

DF 12.5 Wed 9:30 P5

Dielectric and magnetic properties of $CuIn_{1-x}Cr_xP_2S_6$ single crystals — •Vladimir Shvartsman[1], Pavel Borisov[1], Yulian Vysochanskii[2], and Wolfgang Kleemann[1] — [1]Angewandte Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — [2]Institute of Solid State Physics and Chemistry of Uzhgorod University, Ukraine

A variety of electric dipolar arrangements have been recently found in the layered thiophosphate compounds $A^IB^{III}P_2S_6$ (A^I and B^{III} are mono- and trivalent metal ions). In particular, $CuInP_2S_6$ is in a ferrielectric state below 310 K, while $CuCrP_2S_6$ is antiferroelectric below 150 K. The latter compound undergoes also a transition into an antiferromagnetic state at 30 K. We report on investigations of magnetic and dielectric properties of solid solutions between these two compounds, $CuIn_{1-x}Cr_xP_2S_6$ (x = 0.2 - 0.6). Temperature and frequency dependencies of the dielectric permittivity were measured. The distribution of relaxation times has been evaluated from the dielectric spectra. A transition into dipolar glassy state has been revealed below 50 K. The magnetic behavior of these compounds and a possible magnetoelectric coupling are discussed.

DF 12.6 Wed 9:30 P5

Influence of pressure on the ferroelectric phase transition temperature and domain structure in monoclinic $Sn_2P_2S_6$ — •Konstantin Rushchanskii[1] and Yulian Vysochanskii[2] — [1]Institut für Festkörperforschung and Institute for Advance Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Institute for Solid State Physics and Chemistry, Uzhgorod National University, 54 Voloshyn St., 88000 Uzhgorod, Ukraine

Monoclinic $Sn_2P_2S_6$ is a proper uniaxal ferroelectric, a promising material for thermal and acoustic transducers as well as for fast holography and nonlinear optics. High polarizability of the chalcogenide anion sublattice and low crystalline symmetry of this compound allow many interesting phenomena such as coexistance of high and low-symmetry phases, low temperature non-Debye dielectric dispersion, displacive vs order-disorder crossover, relaxation processes near transition point, non-linear soft-mode interactions, etc. In our recent work (Phys. Rev.

Lett. **99**, 207601 (2007)) we developed an *ab initio* model of the temperature driven phase transition in this crystal, which explains most of the experimentally observed phenomena in this system. Moreover, we have found that a domain wall undergoes transformation between metastable smooth-shape configuration to a stable sharp-shape one at low temperatures of around 60 K. In the present contribution we investigate the influence of temperature and pressure on the structure of domain walls. We will show that smooth-shape domain structure is stabilized by high pressure which affects the pressure dependence of the ferroelectric transition temperature.

DF 12.7 Wed 9:30 P5

***Ab initio* characterization of lattice instability in $Eu_{1-x}Ba_xTiO_3$ multiferroics** — •Konstantin Rushchanskii[1], Marjana Ležaić[1], and Nicola Spaldin[2] — [1]Institut für Festkörperforschung and Institute for Advance Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Materials Department, University of California, Santa Barbara, Santa Barbara, CA 93106-5050

It is well known that chemistry of the A-cation in ferroelectric oxides with a perovskite ABO_3 structure influences the lattice strain and is therefore crucial for the structural instability. Incipient ferroelectrics can be turned to the real ones under negative pressure which in bulk systems can be achieved in solid solutions between chemically related compounds. According to recent observations, similar behavior is observed in a solid solution of EuTiO3 and BaTiO3 perovskite oxides. While pure $EuTiO_3$ is a quantum paraelectric which also exhibits antiferromagnetic properties, mixed $Eu_{1-x}Ba_xTiO_3$ compound turns out to be ferroelectric at $x > 0.2$.

We have studied the role of Eu cations on the lattice instability in negatively strained $EuTiO_3$ and ordered $Eu_{1-x}Ba_xTiO_3$ compounds for $x > 0.2$. We have found a significant Eu off-centering both in the mixed compounds and in pure $EuTiO_3$. The influence of hydrostatic pressure on polarization in $Eu_{1-x}Ba_xTiO_3$ have also been studied, which allowed us to derive a phonon picture of the observed Eu cation off-centering together with its detailed electronic structure view.

DF 12.8 Wed 9:30 P5

Influence of commensurability energy on the incommensurate structure dynamics in $[N(CH_3)_4]_2CuCl_4$ crystal — •Ivan Karpa — Ivan Franko Lviv National University, Department of Electronics, Non-linear Optics Chair

Investigations of sample size of $[N(CH_3)_4]_2CuCl_4$ crystal influence on the optical birefringence is studied. It has been shown that decreasing of crystal size is accompanied by increasing of commensurability energy. It is seen in the increasing of incommensurate-commensurate phase transition temperature and expansion of temperature interval of metastable phase existence. It has been set that decreasing of crystal size is accompanied by decreasing of incommensurability parameter. It is seen in the increasing of parent-incommensurate phase transition temperature.

DF 12.9 Wed 9:30 P5

Site-selective determination of coordination symmetries by anisotropic anomalous X-ray scattering — •M. Zschornak[1,2], T. Leisegang[1], H. Stöcker[1], T. Weissbach[1], S. Gemming[2], and D.C. Meyer[1] — [1]Institute of Structural Physics, TU-Dresden, 01062 Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, FZ Dresden-Rossendorf, 01328 Dresden, Germany

Based on an experiment of Kirfel and Petcov on rutile (136) $P4_2/mnm$, which verified anisotropic anomalous scattering (AAS) by measuring 'Forbidden Reflection near Edge Diffraction' (FRED) at an energy of 4985eV, we aimed to extend the results with allowed reflections to extract more tensor symmetries of the Ti scattering factor tensor f_{ij}. Furthermore we intended to study possible restrictions for atomic site occupation of unknown structures in an identified space group due to these local symmetry relations exemplary for this model structure. The rutile samples investigated were 10x10x1mm^3 wafers in (001), (110) and (111) orientation and Ψ-scans were measured for the reflections 001, 220, 110 and 111. Ti occupies Wyckoff site 2*a*, its tensor symmetry must follow the local symmetry *m.mm* leaving 3 complex elements f_{11}, f_{12}, f_{33}. The measured data show clear evidence of AAS and the 001 FRED and 111 intensities could be fitted to obtain f'_{12} and f''_{12}. Since f_{13} and f_{23} were refined to zero, the positioning of Ti in the unit cell would by inverse symmetry arguments only be consistent with respect to site symmetry on Wyckoff sites *a*, *b*, *e*, *f*, *g* (out of *k*).

DF 12.10 Wed 9:30 P5

Deposition of $(Ba_{0.6}Sr_{0.4})TiO_3$ on conducting $PdCoO_2$ — •Stefan Hirsch[1], Philipp Komissinskiy[1], Xianghui Zhou[2], Claudia Fasel[3], and Lambert Alff[1] — [1]Dünne Schichten, Materialwissenschaft TU-Darmstadt, Darmstadt, Deutschland — [2]Forschungszentrum Karlsruhe, Karlsruhe, Deuschland — [3]Disperse Feststoffe, Materialwissenschaft TU-Darmstadt, Deutschland

$(Ba_{0.6}Sr_{0.4})TiO_3$ is investigated intensively due to its promising properties as a tuneable dielectric material with applications e.g. in tunable filters, multi band antennas and high frequency components. High quality $(Ba_{0.6}Sr_{0.4})TiO_3$ (abbreviated: BST60) thin films were grown on $SrTiO_3$ and $NdGaO_3$ substrates by pulsed laser deposition. The powder for the BST60 target was produced by two methods, sol-gel process and by solid state procedure. For the solid state method a thermo gravimetric analysis and differential thermal analysis was made to find the ideal calcination temperatures. All steps were analyzed using X-ray diffraction of the powders and the final target. In the next step a multilayer structure of $PdCoO_2$ as a conductive layer and BST60 on top as a dielectric one is grown by pulsed laser deposition. The powder for $PdCoO_2$ was also produced by a solid state procedure from $PdCl_2$ and CoO. The films were characterized by X-ray diffraction, high resolution scanning electron microscope, ellipsometry and four-point-measurement in the MHz and GHz range. The authors thank DFG GK 1035.

DF 12.11 Wed 9:30 P5

A model of ferroelectricity in thiourea — •Izabela Sliwa[1] and Wojciech Wanarski[2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland — [2]Faculty of Physics, Adam Mickiewicz University, Poznan, Poland

We propose a new mechanism of the phenomenon of ferroelectricity in the molecular crystal of thiourea ($SC(NH_2)_2$). The mechanism is based on a model of interaction between two electric dipoles in molecules. The dipoles are assumed to be not ideal points, but they have a finite length. Besides, they can reorient mutually. The reorientation is determined by the crystal structure specified by experimental structural research. On the basis of this theory, a formula for the potential energy of the interaction of the pair of two non-point dipoles as a function of the angle of reorientation is derived and discussed. The formula is applied within the limit of the molecular field approximation (MFA). We discovered different possible mechanisms of formation of the resultant dipole moments of pairs of molecules which are related to different phases of thiourea monocrystal.

DF 12.12 Wed 9:30 P5

Radioluminescence Investigations on Alumosilicates for Age Determination — •Susanne S. Pfeifer and Matthias R. Krbetschek — Saxon Academy of Sciences, Quaternary Geochronology Section, Inst. of Appl. Physics, TU Freiberg, Leipziger Str. 23, D-09599 Freiberg/Sa., Germany

Age determination of geological and archaeological objects using luminescence phenomena follows the basics of solid state dosimetry of ionising radiation. Luminescence capability is created due to the interaction of radiation with the crystal lattice by charge trapping at defect sites. This metastable state can be built up and last over geological periods and read-out by luminescence stimulation. As the radiation field is created by the decay of natural radioisotopes there is a time dependence of the luminescence signal. Feldspars (alumosilicates) are beside quartz mostly used in luminescence dating of young rocks and artefacts. We carried out radioluminescence investigations on such minerals: i) To determine their potassium concentration (as internal 40K is a main contributor to the radiation field) based on a peak-shift phenomenon in the far-red spectral range (700-750 nm), which allows concentration determination on very small sample amounts. ii) To achieve radioluminescence dating on single mineral grains (200-300 μm) by spatially resolved measurements so that sample inhomogeneities (defect distribution) can be observed more in detail. The latter is based on a newly developed EMCCD camera measurement system. Hence, a wider age range of the IR-radiofluorescence dating method and higher precision of age data for Archaeology and Quaternary Geology will be achieved.

DF 12.13 Wed 9:30 P5

Microstructure control in PZT/(111)-Pt heterostructures — •Salah Habouti[1], Claus-Henning Solterbeck[1], Vladimir Zaporojtchenko[2], Franz Faupel[2], and Mohammed Es-Souni[1] — [1]Institute for Materials and Surface Technology, University of Ap-

plied Sciences Kiel — [2]Chair for Multicomponent Materials, Christian-Albrechts-Universtät zu Kiel

Investigations of film formation of $Pb(Zr_{0.52}Ti_{0.48})O_3$ (PZT) on Pt (111) shows that an interfacial intermetallic layer, Pt_xPb, forms as well under oxidizing and reducing atmosphere when the films are subjected to an intermediate annealing step at 550°C. The formation of the intermetallic layer controls further crystallization and growth of the perovskite phase and confers to it a pronounced (111) texture at the fairly low annealing temperature of 600°C. The crystallization of the morphotropic PZT phase is shown to initiate via incipient formations of a Ti-rich tetragonal phase at the interface with the intermetallic interfacial layer. The results are discussed in terms of thermodynamics and kinetic of phase formation.

DF 12.14 Wed 9:30 P5

Messung der piezoelektrischen Eigenschaften von keramischen Einzelfasern — •Ralf Steinhausen[1], Sabine Kern[1], Christoph Pientschke[1], Horst Beige[1], Frank Clemens[2] und Juliane Heiber[2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Deutschland — [2]EMPA Dübendorf, Schweiz

Piezoelektrische keramische Fasern mit Durchmessern von wenigen 100 μm können in Ultraschallwandlern und mikromechanischen Systemen eingesetzt werden. Die Bestimmung der dielektrischen und piezoelektrischen Eigenschaften erfolgt meist durch Einbetten der Fasern in eine Polymermatrix und anschliessende Bestimmung der Kompositeigenschaften.

Es wurde eine neue Methode auf der Basis eines kapazitiven Sensors entwickelt, mit der die piezoelektrischen Eigenschaften einzelner keramischer Fasern bestimmt werden können. Neben den Dehnungs-Feldstärke-Kurven bei großen Feldstärken und Frequenzen bis 10 Hz kann vor allem auch der lineare piezoelektrische Koeffizient d_{33} der Faser bei kleinen Anregungsspannungen bestimmt werden. Die Methode wurde zur Charakterisierung von PZT-Fasern mit Durchmessern von 250 μm verwendet.

DF 12.15 Wed 9:30 P5

Spektrale Untersuchungen im mmW und sub-mmW-Bereich für industrielle Anwendungen der Qualitätskontrolle — •Gört Oliver Luedtke[1], Klaus Wandelt[1] und Dirk Nüssler[2] — [1]Institut für Theoretische u. Physikalischee Chemie, Wegelerstr. 12, 53115 Bonn — [2]FGAN-FHR, Abt. MHS, Neuenahrer Str 20, 53343 Wachtberg

Die kontinuierliche Kontrolle von Produktionsabläufen stellt eine große Herausforderung für moderne Messverfahren dar. Neben der Detektion von Verunreinigungen in Produkten sind auch die Überwachung und Nachjustierung von Prozessparametern eine wesentliche Anforderungen an die Produktionskontrolle. Im Gegensatz zu der Überwachung der reinen physikalischen Größen, geht es bei den Messverfahren um die fortlaufende Kontrolle am Produkt. Die in Echtzeit durchgeführte Qualitätskontrolle, erlaubt die Verwendung wesentlich geringerer Toleranzbereiche im Herstellungsprozess. Hierbei müssen Bewertungskriterien untersucht werden, die aus den gemessenen Größen die Steuerparameter für den Produktionsprozess ableiten. Die Integration von spektralen mmW und sub-mmW Untersuchungsmethoden in Produktionsabläufe erfordert dabei die Berücksichtigung sehr unterschiedlicher physikalischer Einflüsse. Neben makroskopischen Effekten wie Mehrfachreflektionen, Brechungsindizes oder Beugungs- und Streueffekte sind Gruppeneffekte, wie die Absorptionslinien unterschiedlicher Stoffe, wesentliche Ansatzpunkte eines Analyseverfahrens. Die vorgestellte Arbeit beschreibt die unterschiedlichen Einflüsse und zeigt an konkreten Beispielmessungen, wie entsprechende Effekte zur Produktionsüberwachung genutzt werden können.