DF 15: Optical and Nonlinear Optical Properties II (DF with KR)

Time: Wednesday 15:00–17:40 Location: EB 407

DF 15.1 Wed 15:00 EB 407

Local defect structure and dielectric relaxation in $LiNbO_3$ single crystals — Guillaume F. Nataf, Nadège Meyer, and •Torsten Granzow — Luxembourg Institute of Science and Technology (LIST), Belvaux, Luxembourg

The defect structure of $LiNbO_3$ (LN) has been studied more extensively than that of most other oxide ferroelectrics for several reasons. First, congruently melting LN is already rich in defects: it is strongly Li-deficient and contains a high concentration of Nb_{Li} antisite defects. Second, the possibility to adjust the optical properties by doping with a wide range of ions has increased the usefulness of LN for optical applications. Third, due to the high mobility of Li at moderate temperatures, the poling procedure can have a profound influence on the local defect structure. However, few studies have considered the effect of this local structure on the dielectric properties of LN. In this presentation, the temperature dependence of the real and imaginary part of the electrical permittivity of differently doped LN single crystals is investigated in the frequency range from 1 Hz to 1 MHz. Different relaxation phenomena are caused by thermal and electrical treatment and traced to differences in the local defect structure. Ferroelectric domain walls stabilize the local defect structure. These assumptions are supported by measurements of the temperature dependence of electrical conductivity and the thermally stimulated depolarization current.

DF 15.2 Wed 15:20 EB 407

Influence of defects on the ferroelectric and electrocaloric properties of $BaTiO_3$ — •Anna Grünebohm[1] and Takeshi Nishimatsu[2] — [1]Fakultät für Physik, Uni Due, Germany — [2]IMR, Tohoku University and Faculty of Physics, Japan

The electrocaloric effect is an adiabatic temperature change of a material upon applying an external electrical field. Recently, this effect has been rediscovered as a promising candidate for solid state refrigeration as large temperature changes have been found in experiment and theoretical simulations.[1,2,3] However, the underlying mechanisms for the large caloric response as well as possible obstacles are still not well understood. In addition, the effective temperature range in pure ferroelectric materials is narrow. We thus perform molecular dynamics simulations of an ab initio based effective Hamiltonian as implemented in the *feram* package[3] in order to study the effect of defects, strain, and alloying on the electrocaloric response and its operation range.

[1] A. Mishenko, *et al*, Science **311**, 1270 (2006)
[2] I. Ponomareva *et al*, Phys. Rev. Lett. **108**, 167604 (2012)
[3] T. Nishimatsu *et al*, J. Phys. Soc. Jpn., **82**, 114605 (2013)

DF 15.3 Wed 15:40 EB 407

Probing of local polarization dynamics in uniaxial SrxBa1-xNb2O6 single crystals — •Vladimir Shvartsman[1], Jan Dec[2], Sergei Kalinin[3], Wolfgang Kleemann[4], and Doru Lupascu[1] — [1]Institute for Materials Science, University Duisburg-Essen, Essen, Germany — [2]Institute of Materials Science, University of Silesia, Katowice, Poland — [3]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, USA — [4]Faculty of Physics, University Duisburg-Essen, Duisburg, Germany

Unique properties of relaxor ferroelectrics are to a great extent determined by dynamics of the local polarization. In these materials only short range polar order exists inside so called polar nanoregions (PNRs). Being dynamic at high temperatures, PNRs are "frozen" below certain critical temperature forming a glassy-like state.

Here we report on our recent piezoresponse force microscopy (PFM) investigations of local polarization dynamics in SrxBa1-xNb2O6 (SBN100x) single crystals. The temperature dependent PFM studies of relaxors SBN75 and SBN80 revealed appearance of static PNRs already far above the freezing temperature. These static PNRs coexist with still dynamic those in a broad temperature interval. The response from dynamic PNRs was probed by studying the temporal decay of local piezoresponse after excitation by an electric field pulse. A mapping of relaxation parameters has been performed to reveal spatial heterogeneity of the polarization dynamics. The effect of temperature and composition on the local polarization dynamics has been analyzed.

DF 15.4 Wed 16:00 EB 407

Multiphoton-induced luminescence and its domain contrast in Mg-doped $LiNbO_3$ and $LiTaO_3$ — •Philipp Reichenbach[1], Thomas Kämpfe[1], Andreas Thiessen[1], Alexander Haussmann[1], Robin Steudtner[2], Theo Woike[3], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George- Bähr-Str. 1, 01069 Dresden, Germany, 01069 Dresden, Germany — [2]Institut für Ressourcenökologie, Helmholtz-Zentrum Dresden, Bautzner Landstraße 400, 01328 Dresden — [3]Institut für Strukturphysik, Technische Universität Dresden, Zellescher Weg 16, 01069 Dresden, Germany

Mg doped $LiNbO_3$ (LNO) and $LiTaO_3$ (LTO) emit a spectrally broad multiphoton luminescence upon excitation with tightly-focused ultrashort laser pulses centered at 2.5 eV [1,2]. Time-resolved acquisition reveals a stretched exponential decay of the photoluminescence, which confirms the luminescence to stem from recombination of electron and hole polarons. Furthermore, the luminescence also shows a distinct contrast between virgin and single inverted domains of about 3% and 20 - 30% for LNO and LTO, respectively [2]. LNO exhibits the same contrast value when thermally pretreated at 1000°C under oxygen atmosphere before poling. The contrast decays thermally-excited above 100°C with an activation energy around 1 eV for both LNO and LTO. This indicates the contrast and its decay to be strongly connected to the lithium ion concentration and their activation.

[1] P. Reichenbach et al., J. Appl. Phys. 115, 213509 (2014)
[2] P. Reichenbach et al., Appl. Phys. Lett. 105, 122906 (2014)

DF 15.5 Wed 16:20 EB 407

Extended *ab-initio* study of the $LiNbO_3$ band gap — •Arthur Riefer, Simone Sanna, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33098 Paderborn

Lithium niobate ($LiNbO_3$) is one of the most important ferroelectric materials and the most important nonlinear optical material. The electronic and optical properties of $LiNbO_3$ have been studied in recent years with *ab-initio* methods [1-4] within high accuracy indicating good agreement with experimental results. However, measurements by Redfield *et al.* [5] show a temperature dependence of the band gap, which can be traced back to different effects. In order to model the temperature dependence of the electronic band gap, we have extended the approaches described in Refs. [1-4] under two aspects. On the one hand, hybrid functionals are employed to provide improved starting points for many-body perturbation theory, which is applied to study the electronic properties. On the other hand, the influence of the temperature on the $LiNbO_3$ band gap is investigated by means of molecular dynamics simulations. The results are compared with former works and experimental findings.

[1] W. G. Schmidt *et al.*, Phys. Rev. B **77**, 035106 (2008)
[2] C. Thierfelder *et al.*, phys. stat. sol. (c) **7**, 362 (2010)
[3] A. Riefer *et al.*, IEEE Trans. on Ultrasonics, Ferroelectrics and Frequency Control **59**, 1929 (2012).
[4] A. Riefer *et al.*, Phys. Rev. B. **87**, 195208 (2013)
[5] Redfield *et al.*, J. Appl. Phys. **45**, 10, (1974)

DF 15.6 Wed 16:40 EB 407

Structural characterization of substituted lanthanum tungstates with X-Ray and Neutron Diffraction — •Andrea Fantin[1], Tobias Scherb[1], Gerhard Schumacher[1], Janka Seeger[2], and Wilhelm A. Meulenberg[2] — [1]Helmholtz-Zentrum Berlin für Materialen und Energie, Hahn-Meitner-Platz 1, D-14109 Germany — [2]Forschungszentrum Jülich, D-52425 Jülich, Germany

Our work on proton conducting materials deals with structural characterization of two different series of substituted lanthanum tungstates: La5.4W(1-x)MxO12-delta with M=Mo,Re and 0<=x<=0.2. The main methods used to understand their crystal structure are Neutron Diffraction (ND) and High-Resolution X-Ray Diffraction (HRXRD). Experiments were carried at ILL (Grenoble, France) and PSI (Villigen, Switzerland). Different elemental contrast is reached with these complementary diffraction techniques.

Our specimens consist of three cations (La, W, Mo or Re) and oxygen anions. In order to distinguish W (Z=74, b=4.86fm) and Re (Z=75, b=9.2fm) neutrons are needed, while for La (Z=57, b=8.2fm), W(Z=74, b=4.86fm) and Mo (Z=42, b=6.7fm) good contrast is also given by X-Rays. Combined refinements to model accurately anti-

site disorder, position of the substituted elements and oxygen (Z=8, b=5.8fm) positions in this highly disordered material are mandatory.

Measurements in dependence of temperature down to 1.5K confirm the structural model suggested by one of the coauthors without any unmodeled static disorder. Substitution and deuteration/humidification show no relevant structural changes.

DF 15.7 Wed 17:00 EB 407

Structure Solution and Prediction for Complex Modular Materials — •Kathryn Bradley, Matthew Dyer, Christopher Collins, John Claridge, George Darling, and Matthew Rosseinsky — Department of Chemistry, University of Liverpool, Liverpool, L69 7ZD, United Kingdom

Complex functional transition metal oxides can generally be described in terms of layers or modules containing elements in particular chemical environments. This observation has led to the development of the Extended Module Materials Assembly (EMMA) approach for the generation of plausible candidate structures of particular compositions. Combining the modular description with classical lattice dynamics and structure optimization with DFT, the EMMA method has recently been extended to study hexagonal perovskite structures, exploring the family of B-site deficient barium cobalt niobates.[1]

[1] K. Bradley et al., Phys. Chem. Chem. Phys., 2014,16, 21073-21081. DOI: 10.1039/C4CP01542H

DF 15.8 Wed 17:20 EB 407

Perspectives for photorefractive materials in neutron physics — •Romano Rupp[1], Martin Fally[1], Jürgen Klepp[1], Christian Pruner[2], Yasuo Tomita[3], and Irena Drevensek[4] — [1]Univ. Wien, Austria — [2]Univ. Salzburg, Austria — [3]University of Electro-Communications, Tokyo, Japan — [4]Univ. Ljubljana and Josef-Stefan-Institute Ljubljana, Slovenia

The phenomenon where light irradiation changes the refractive index is called a photorefractive effect. There are several mechanisms that may result in neutron photorefraction. For example, all photoconductive isolators have in principle the potential to exhibit neutron photorefraction. Particularly strong effects appear in piezoelectric materials, mixed electronic-ionic conductors or materials close to, e.g., a ferroelectric phase transition. We report on neutron diffraction from holographic gratings induced by light irradiation, neutron-induced holographic grating decay, and investigations on light-sensitive dielectrics and nanoparticle composites for applications in neutron physics.