DF 13: Poster II: Electrical, mechanical and optical properties, nonlinear dielectrics

Time: Wednesday 15:00–17:30 Location: Poster A

DF 13.1 Wed 15:00 Poster A

Barrier heights, polarization switching and electrical fatigue in PZT ceramics with different electrodes — •Andreas Klein, Jürgen Rödel, Heinz von Seggern, Torsten Granzow, Feng Chen, Sergey Zukov, Robert Schafranek, Andre Wachau, and Julia Glaum — Technische Universität Darmstadt, Institute of Material Science, Petersenstraße 32, D-64287 Darmstadt, Germany

Metal Pt, transparent conductive oxide ITO (In_2O_3:10at% Sn) and metal oxide RuO_2 were deposited by sputtering on PZT ceramics as electrodes. The Schottky barrier heights at the ferroelectric/electrode interfaces are determined by photoelectron spectroscopy. The barrier heights vary significantly and indicate a preference for either hole or electron injection. The polarization, strain, permittivity, and piezoelectric constant hysteresis loops are, however, identical for all electrodes. Very small changes are observed in the polarization dependence on time and applied field, which was studied over a broad time window ranging from 10^{-7} to 10^2 s for applied fields between 1 and 2 kV/mm. A 20% reduction of polarization after 10^6 bipolar cycling is observed for all the samples. In contrast to PZT thin films, the loss of remanent polarization with bipolar switching cycles does not depend on electrode material, indicating a different fatigue mechanism for thin film and bulk ceramics.

DF 13.2 Wed 15:00 Poster A

Low frequency properties of space-charge wave excitation — •Thomas Schemme, Burkhard Hilling, Kay-Michael Voit, Heinz-Jürgen Schmidt, and Mirco Imlau — Department of Physics, University of Osnabrück, Germany

One possibility for the excitation of space-charge waves (SCW) in semi-insulating materials is the illumination with a superposition of one static and one moving interference pattern with equal spatial frequency and the application of a static electric field [1]. In this case, a constant ac signal at frequencies lower the resonance frequency of the SCW is uncovered. This low frequency signal does not persist using an oscillating pattern for excitation, i.e., it is a particular artefact of the four-beam excitation. To analyze this additional signal, both methods are analyzed comparatively in terms of their light pattern. We discuss the origin of the low frequency signal in the frame of a spatial modulation of the photoconductivity and give experimental evidence for our model approach. Thereby, a brief introduction into the theory describing the SCW-signal is presented. Financial support from the Deutsche Forschungsgemeinschaft within the Graduate College 695 is gratefully acknowledged.

[1] B. Hilling *et al.*, PRB **80**, 205118 (2009)

DF 13.3 Wed 15:00 Poster A

Light-induced linkage isomerization of photochromic $[Ru(bpy)_2(R\text{-}OSO))]^+$ compounds — •Kristin Springfeld[1], Volker Dieckmann[1], Sebastian Eicke[1], Mirco Imlau[1], and Jeffrey J. Rack[2] — [1]Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — [2]Department of Chemistry and Biochemistry, Ohio University, Athens, Ohio 45701

Ruthenium sulfoxides exhibit light-induced linkage isomerization of the SO-bond with remarkable photosensitivity $S = (0.25 \pm 0.03)\,\mathrm{W s\,cm^{-1}}$ and extended lifetimes of the related metastable states in the order of 10^4 s [1]. The isomerization is accompanied with tremendeous changes of the optical extinction up to $9350\,\mathrm{cm^{-1}\,mol^{-1}}$ thus enabling the study of linkage isomerization by means of time-resolved optical spectroscopy. Here, the influence of ligand substitution is studied via inspection of the photosensitivity and the generation and relaxation dynamics of the photochromic response as a function of temperature (pump at $\lambda = 405$ nm , probe at $\lambda = 532$ nm). The spectra of the modified compounds, where ligands R = Bn, BnCl, and BnMe were attached to OSO, were compared with the reference system $[Ru(bpy)_2(OSO))]^+$. It turns out, that the new ligands affect the absorption features and the photosensitivity of the system only slightly. In contrast, a strong influence of the thermal relaxation of the metastable states is uncovered. Remarkably, the influence on the frequency factors is much more pronounced than on the activation energies achieved by Arrhenius' law.

[1] Dieckmann et al., Opt. Express, 17, 15052 (2009)

DF 13.4 Wed 15:00 Poster A

Phototriggered NO and CN release from $[Fe(CN)_5NO]^{2-}$ molecular monolayers attached to TiO_2 surfaces — •Volker Dieckmann[1], Mirco Imlau[1], Dereje Hailu Taffa[2], Lorenz Walder[2], Robert Lepski[3], Dominik Schaniel[3], and Theo Woike[3] — [1]Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — [2]Institute of Chemistry, Universtity of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — [3]I. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Phototriggered NO and CN release from $[Fe(CN)_5NO]^{2-}$ (NP) molecular monolayers is studied by a combination of electrochemistry, infrared spectroscopy, and mass spectrometry under light exposure at temperatures of 80 K and 294 K. The NP molecular monolayers were electrostatically attached to thin films of mesoporous TiO_2 deposited on silicon. Irradiation of the surfaces results in NO and CN release, which is verified with mass spectrometry. The kinetics of the NO release are determined by inspection of the ν_{NO} stretching mode as a function of exposure to light in the violet/green spectral range. The decrease of the ν_{NO}-amplitude can be modeled considering the NO release as a two-step process with an intermediate state between the attached and the released state. According to literature, the intermediate state may be related to the light-induced linkage NO isomerization of the NP. Financial support by the DFG (GRK 695, WO618/8-1), the federal state of Lower Saxony (Lichtenberg-Stipendium) and the BMBF (FKZ 03X5510) is gratefully acknowledged.

DF 13.5 Wed 15:00 Poster A

Time-resolved analysis of short-living mixed phase and amplitude gratings — •Raphael-Sung Hardt, Hauke Bruening, Bettina Schoke, and Mirco Imlau — Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

The time-resolved analysis of short-living mixed phase and amplitude gratings is a demanding challenge in materials with an optical response originating from optically excited, metastable states. For instance, such gratings appear in materials featuring the optical generation of strongly localized charge carriers or photo-induced linkage isomerism in molecular crystals. An established tool for volume grating analysis is the determination of the diffraction efficiency as a function of the angular detuning $\Delta\theta_B$ from the Bragg angle θ_B, i.e., the so-called rocking curve. Fitting of the data set with appropriate functions allows to separate the individual contributions of phase and amplitude gratings to the overall diffraction efficiency and further yields information on a mutual phase shift. With thermally reduced, nominally undoped $LiNbO_3$ as an example we show our results on the time-resolved determination of the rocking curve in the time regime of 10^{-8} s to 10^2 s with a temporal resolution of up to 10 ns. The gratings are recorded by pulsed laser light ($\lambda = 532$ nm, $\tau = 8$ ns) and are probed in the near-infrared spectral range at $\lambda = 785$ nm. Grating analysis yields the temporal development of phase and amplitude gratings, which originate from optically generated small polarons.

*Financial support by the DFG (Projects IM37/5-1 and GRK 695) is gratefully acknowledged.

DF 13.6 Wed 15:00 Poster A

Photonic Band Structure Analysis of Bi- and Multicontinuous Structures — •Matthias Saba and Gerd Schröder-Turk — Institut für Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr. 7B, 91058 Erlangen, Germany

Photonic crystals based on triply-periodic minimal surfaces have recently attracted attention because of their occurence in biological systems, e.g. in butterfly scales or beatle shells. Here we analyse the photonic band structure of bicontinuous surface models (dividing space into two intertwined continuous network domains) and multicontinuous surface models (with three or more continuous network domains), with and without chirality, that are models for self-assembled biological or chemical structures. Triply-periodic surfaces with constant mean curvature H_0 are generated by numerical minimization of a surface energy functional $\int dS(H(r) - H_0)^2$. One or more of these surfaces divide space into interpenetrating networks which are filled with materials of different dielectric constants. The band structures of the resulting bi- and multicontinuous photonic crystals are computed by

the frequency domain eigensolver MPB. The aim of this work is to find structures with complete band gaps.

DF 13.7 Wed 15:00 Poster A

Metamaterial hydrogen sensor — •Patrick Mai and Harald Giessen — 4. Physikalisches Institut, Universität Stuttgart

Hydrogen has gained a substantial amount of interest in recent years and is considered to be a future carrier of energy. However, hydrogen can mix and ignite with air in a wide concentration range - hence monitoring is necessary.

We present an optical hydrogen sensor based on a metamaterial principle. Our stacked sample consists of a gold mirror and palladium nanowires. By tailoring the structural parameters one can tailor the optical properties and achieve a hydrogen-dependent response.

We present temperature- and time-dependent measurement results. Advantages and disadvantages over conventional hydrogen sensors are pointed out, and the development towards an all-optical hydrogen sensor with full seperation of detection electronics and measurement optics will be discussed.

DF 13.8 Wed 15:00 Poster A

Raman scattering of $BiCrO_3$ thin films: experimental and first-principles studies — •Cameliu Himcinschi[1], Ionela Vrejoiu[2], Silvia Schumann[1], Christian Röder[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

The strong research interest in multiferroic epitaxial films arises from their interesting properties and is stimulated by their potential applications in non-volatile ferroelectric memories or novel multiple state memories and devices based on magnetoelectric effects. Among the Bi-containing perovskite-type transition metal oxides, $BiCrO_3$ is the least investigated one and the literature is still lacking Raman scattering data. In this work epitaxial thin films of $BiCrO_3$ were deposited onto $NdGaO_3$ (110) substrates by pulsed laser deposition. Bulk $BiCrO_3$ has a monoclinic structure with the space group C2/c below 420 K [1]. The Raman spectra of the $BiCrO_3$ films were measured from 77 K to room temperature using a UV Labram spectrometer. The 325 nm emission line of a HeCd laser was used for excitation. The assignment of the phonon modes in the Raman spectra of $BiCrO_3$ was done by comparing the experiments with density functional theory calculations.

[1] A.A. Belik *et al.*, Chem. Mater 20, 3765 (2008).

DF 13.9 Wed 15:00 Poster A

Ab initio study of phonons in $BaTiO_3$ — •Pavel Ignatiev and Valery Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Ferroelectric $BaTiO_3$ ceramic is a very important technological material. Its structure, however, can be different from the perovskites ideal cubic phase. Depending on temperature $BaTiO_3$ can turn to rhombohedral, orthorhombic, tetragonal, cubic and even hexagonal phases. Here we present an ab initio study of various phases of BaTiO3. We report on the optimized lattice parameters, electronic structure and phonons. Ab initio calculations are performed by means of the density functional theory implemented in Quantum Espresso package [1]. Phonons are calculated using the density functional perturbation theory [2]. Polarization-induced LO/TO splitting of phonon branches and Born effective charge tensors are obtained from the first principles using modern polarization theory.

[1] P. Giannozzi et al., J. Phys.: Condens. Matter 21, 395502 (2009).
[2] S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, Rev. Mod. Phys. 73, 515 (2001).

DF 13.10 Wed 15:00 Poster A

thermisches Polarisationsrauschen von Silbernatriumnitrit — •Jumna Mehlis — Martin-Luther-Universität Halle-Wittenberg, Halle(Saale), Germany

Messung des thermischen Polarisationsrauschspektrums in der Umgebung des strukturellen Phasenüberganges eines ferroelektrischen Silbernatriumnitrit-Kristalles

DF 13.11 Wed 15:00 Poster A

The influence of external electric fields on ferroelectric domain lengths in Calcium Barium Niobate — •Urs Heine[1], Klaus Betzler[1], Manfred Burianek[2], and Manfred Muehlberg[2] — [1]Department of Physics, University of Osnabrueck, D-49069 Osnabrueck — [2]Institute of Crystallography, University of Cologne, D-50674 Cologne

We present optical investigations on the novel tungsten bronze type Calcium Barium Niobate (CBN). Using the Czochralski method, [001]-oriented colorless single CBN crystals were grown from the congruently melting composition of 28.1 mole% calcium. The samples with 12 mm in diameter and about 80 mm in length were cut to 2 - 5 mm thickness, and the c-faces were polished to optical quality. Water electrodes were used to connect the c-faces to a high voltage supply, while simultaneously directing an infrared laser beam parallel to the c-axis. When illuminating the crystal, a conical light pattern emerges from the back side of the crystal due to quasi-phase matched second harmonic generation (SHG). The size distribution of the ferroelectric domain structure, contributing to the quasi-phase matching process, manifests itself in the angular intensity distribution of the SHG light pattern. We investigated the field dependent angular intensity distribution, which allows for calculating back on the average domain size, and in particular the mean length of the ferroelectric domains. The influence of ferroelectric aging effects on the domain length was also observed. Monte Carlo simulations were used for fitting generated domain structures with particular mean domain widths and lengths to the measurement data.

DF 13.12 Wed 15:00 Poster A

The local structure of 0.9PZN-0.1PT at high temperature and pressure — •Naemi Waeselmann[1], Boriana Mihailova[1], Bernd Maier[1], Marin Gospodinov[2], and Ulrich Bismayer[1] — [1]Institute of Mineralogy and Petrology, University of HAmburg, Gindelallee 48, D-20146 Hamburg, Germany — [2]Institute of Solid State Physics, Bulgarian Academy of Science, Blvd. Tzarigradsko Chausse 72, 1784 Sofia, Bulgaria

Single crystals of (1-x)$Pb(Zn_{1/3}Nb_{2/3})O_3$ (PZN)-$x$$PbTiO_3$ (PT) show extremely strong direct and converse piezoelectric effect and are considered as one of the most promising materials for next generation electromechanical sensors and transducers. Solid solutions of (1-x)PZN-xPT with a low x-value exhibit rhombohedral symmetry, whereas those with a high x-value have a tetragonal structure, and the morphotropic phase boundary (MPB) is found to be near $x = 0.1$. In situ high-pressure and high-temperature Raman scattering data on 0.9PZN-0.1PT are analysed in order to give a better insight into the atomic arrangements in the vicinity of MPB.