

## Dielectric Solids Division Fachverband Dielektrische Festkörper (DF)

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### Overview of Invited Talks and Sessions (lecture rooms HSZ 401, WIL A 317, WIL B 321, and Poster P5)

#### Invited Talks

DF 3.1	Mon	14:30–15:00	WIL A317	<b>Interaction of molecules with dielectric surfaces: From single molecular adsorption to functional devices</b> — ●LUKAS M. ENG
DF 3.5	Mon	16:10–16:40	WIL A317	<b>Fluorescence and ordering of aromatic molecules on thin dielectric films</b> — ●MORITZ SOKOLOWSKI
DF 4.1	Mon	10:00–10:35	WIL B321	<b>Magnetoelectric effects and excitations in multiferroic manganites</b> — ●ANDREI PIMENOV
DF 7.1	Tue	14:00–14:35	WIL A317	<b>Origins of large piezoelectric response and lead-free alternatives to PZT</b> — ●DRAGAN DAMJANOVIC
DF 10.1	Wed	10:00–10:35	WIL A317	<b>Photoswitchable Complexes: Properties and Applications</b> — ●DOMINIK SCHANIEL
DF 11.1	Wed	14:30–15:05	WIL A317	<b>Real-time probing of structural dynamics in perovskite materials</b> — ●THOMAS ELSAESSER
DF 14.1	Thu	10:00–10:35	WIL A317	<b>Spatial nonlinear optics in photonic crystals</b> — ●DETLEF KIP
DF 16.1	Thu	14:30–15:05	WIL B321	<b>Simulation of Defects and Domain Structures in Ferroelectrics</b> — ●RALF MÜLLER

#### Tutorial: Multiferroics and Magnetoelectrics

Organisation: Wolfgang Kleemann

DF 1.1	Sun	16:00–16:45	HSZ 401	<b>Magnetic and ferroelectric materials</b> — ●WOLFGANG KLEEMANN
DF 1.2	Sun	16:50–17:35	HSZ 401	<b>Magnetoelectric coupling in multiferroics: Recent developments</b> — ●MANFRED FIEBIG
DF 1.3	Sun	17:40–18:30	HSZ 401	<b>Multiphase multiferroics</b> — ●KATHRIN DÖRR

#### Focus Session: Interaction of Molecules with Dielectric Surfaces

Organisation: Angelika Kühnle

DF 3.1	Mon	14:30–15:00	WIL A317	<b>Interaction of molecules with dielectric surfaces: From single molecular adsorption to functional devices</b> — ●LUKAS M. ENG
DF 3.2	Mon	15:05–15:25	WIL A317	<b>Studying terephthalic acid on dielectric surfaces using non-contact atomic force microscopy</b> — ●PHILIPP RAHE, MARKUS NIMMICH, ANGELIKA KÜHNLE
DF 3.3	Mon	15:25–15:45	WIL A317	<b>Theoretical contributions to the characterization of adsorbates at titania surfaces</b> — ●THOMAS BREDOW
DF 3.4	Mon	15:45–16:05	WIL A317	<b>Accurate Energetics of Ground and Excited States of Molecules on Surfaces</b> — ●THORSTEN KLÜNER
DF 3.5	Mon	16:10–16:40	WIL A317	<b>Fluorescence and ordering of aromatic molecules on thin dielectric films</b> — ●MORITZ SOKOLOWSKI
DF 3.6	Mon	16:40–17:00	WIL A317	<b>Determination of Molecule Orientation on Oxide Surfaces by Near-Edge X-ray Absorption Spectroscopy</b> — ●ALEXEI NEFEDOV, MIKHAIL NABOKA, CHRISTOF WÖLL

DF 3.7 Mon 17:00–17:20 WIL A317 **Adsorption of Organic Molecules on Moderately Reactive Substrates** — •MICHAEL ROHLFING, ANDREAS GREULING, THOMAS BREDOW

### Symposium SYAI: Ab-Initio Approaches to Excitations in Condensed Matter

See SYAI for the full program of the Symposium.

#### Sessions

DF 1.1–1.3	Sun	16:00–18:30	HSZ 401	<b>Tutorial: Multiferroics and Magnetoelectrics</b>
DF 2.1–2.7	Mon	10:40–13:00	WIL A317	<b>Dielectric Spectroscopy &amp; Microscopy</b>
DF 3.1–3.7	Mon	14:30–17:20	WIL A317	<b>Focus Session: Interactions of Molecules with Dielectric Surfaces</b>
DF 4.1–4.7	Mon	10:00–12:40	WIL B321	<b>Multiferroics, Phase Transitions &amp; Relaxors</b>
DF 5.1–5.6	Mon	15:00–17:00	WIL B321	<b>High-k and low-k Dielectrics</b>
DF 6.1–6.16	Tue	9:30–12:30	P5	<b>Poster I</b>
DF 7.1–7.6	Tue	14:00–16:20	WIL A317	<b>Advanced Dielectrics</b>
DF 8.1–8.8	Tue	10:00–12:40	WIL B321	<b>Glass I</b>
DF 9.1–9.6	Tue	14:00–16:00	WIL B321	<b>Glass II</b>
DF 10.1–10.7	Wed	10:00–12:40	WIL A317	<b>Photonic Dielectrics I</b>
DF 11.1–11.7	Wed	14:30–17:10	WIL A317	<b>Photonic Dielectrics II</b>
DF 12.1–12.15	Wed	9:30–12:30	P5	<b>Poster II</b>
DF 13.1–13.7	Wed	14:40–17:00	WIL B321	<b>Thin Films and Nanostructures I</b>
DF 14.1–14.8	Thu	10:00–13:00	WIL A317	<b>Photonic Dielectrics III</b>
DF 15.1–15.7	Thu	10:40–13:00	WIL B321	<b>Thin Films and Nanostructures II</b>
DF 16.1–16.5	Thu	14:30–16:30	WIL B321	<b>Thin Films and Nanostructures III</b>

### Annual General Meeting Dielectric Solids Division

Mittwoch 17:30–18:30 Raum WIL A 317

- Bericht des Fachverbandsleiters
- Tagungsnachlese
- Eingeladene Vorträge 2010
- Tutorial, Focus Sessions und Symposia 2010
- Verschiedenes

### Annual General Meeting Crystallography Division

Donnerstag 17:00–18:00 Raum WIL B321

## DF 1: Tutorial: Multiferroics and Magnetolectrics

Time: Sunday 16:00–18:30

Location: HSZ 401

**Tutorial** DF 1.1 Sun 16:00 HSZ 401  
**Magnetic and ferroelectric materials** — •WOLFGANG KLEEMANN — Angewandte Physik, Universität Duisburg-Essen, Lotharstr.1, 47048 Duisburg, Germany

In this introductory lecture, pertinent examples, mechanisms and basic theories of magnetic and ferroelectric phase transitions will be presented. We discuss the respective ordered states, the domain structures and some functional properties of relevant materials. Owing to their close vicinity to multiferroic and magneto-electric materials, oxidic systems will be brought into focus.

## 5 min. break

**Tutorial** DF 1.2 Sun 16:50 HSZ 401  
**Magnetolectric coupling in multiferroics: Recent developments** — •MANFRED FIEBIG — HISKP, Universität Bonn, Bonn, Germany

Currently, an enormous interest in multiferroics – compounds uniting two or more forms of primary ferroic ordering in one phase – is observed. Aside from technological aspects the interplay of different forms of (anti-) ferroic ordering is a rich source for exploring the fundamental science of phase control. Magnetic ferroelectrics may constitute the most interesting type of multiferroics because they may exhibit an unusually strong, so-called magnetolectric (ME), coupling of magnetic and electric properties which is useful for controlling magnetic order with electric fields and vice versa. In my talk I will discuss the intricate relation between multiferroicity, ME behavior, and symmetry in ME single-phase multiferroics with particular emphasis on recent developments. For example, simultaneous breaking of time- and space-inversion symmetry by magnetic spirals leads to a new type of “induced” ME multiferroic observed, e.g., in orthorhombic RMnO<sub>3</sub>,

pyroxenes, or MnWO<sub>4</sub>. This has to be distinguished from multiferroicity in the popular compound BiFeO<sub>3</sub> which also forms spin-spirals, but independent of the ferroelectric order. On the other hand, space-time asymmetry can also lead to ferrotoroidicity (a spontaneous order of magnetic vortices) as an entirely different form of ferroic ordering observed, e.g., in LiCoPO<sub>4</sub>.

## 5 min. break

**Tutorial** DF 1.3 Sun 17:40 HSZ 401  
**Multiphase multiferroics** — •KATHRIN DÖRR — IFW Dresden, Postfach 270116, 01171 Dresden, Germany

This tutorial addresses multiferroic materials and devices comprising two or more ferroic (ferroelectric or magnetic) phases. Single-phase multiferroics are rare and typically work at low temperatures. A combination of appropriate phases can provide multiferroicity and large magnetolectric coupling also at ambient temperatures, and early applications have been realized.

One crucial issue is how the different ferroic phases must be coupled in order to achieve a large “composite” magnetolectric effect, i. e. the desirable electric control of magnetic order (or magnetic control of dielectric order). The coupling mechanisms by (i) elastic strain and (ii) charge at the interface between the phases will be discussed. Examples for these cases are a piezoelectric-magnetostrictive layered “sandwich” structure and a field-effect transistor with ferroelectric gate and magnetic channel, respectively. The various designs of the composite materials will be followed through history, ending with self-organized and artificially patterned thin film nanostructures. Finally, the most promising approaches known today will be introduced. These include multiferroic sensors for magnetic ac fields, spin-polarized tunnel junctions with multiferroic barrier and the electrically controlled magnetic exchange bias effect from a BiFeO<sub>3</sub> layer.

## DF 2: Dielectric Spectroscopy &amp; Microscopy

Time: Monday 10:40–13:00

Location: WIL A317

DF 2.1 Mon 10:40 WIL A317  
**Space-charge wave spectroscopy of hexagonal silicon carbide** — •MICHAELA LEMMER, BURKHARD HILLING, and MIRCO IMLAU — Department of Physics, University of Osnabrück, Osnabrück, Germany

Space-charge wave (SCW) spectroscopy is based on resonant excitation of SCW in a semi-insulating material, for instance, high resistive semiconductors. This promising new technique allows to examine important photoelectric parameters of a wide variety of materials.

Here, hexagonal silicon carbide with 4H and 6H stacking sequence has been investigated by SCW spectroscopy. For SCW excitation, the sample is exposed to a light pattern oscillating around an equilibrium position. This is realized with a two-beam Mach-Zehnder interferometer, where one of the beams is sinusoidally phase-modulated with an electro-optic phase-modulator. The dispersion behaviours found for the 4H sample indicate the existence of *trap recharging waves* and yield the product of mobility and lifetime  $\mu\tau$  and the effective trap density  $N_{\text{eff}}$ . The data set of the 6H polytype indicates a comparably smaller effective trap density, but an unambiguous assignment to the existence of trap recharging waves fails. Taking into account the general classification of material parameters which provides the existence for SCW, the particular case of *damped, forced charge-density oscillations* can be concluded.

Financial support from the Deutsche Forschungsgemeinschaft (DFG, project Nos. GRK 695 “nonlinearities of optical materials”) is gratefully acknowledged.

DF 2.2 Mon 11:00 WIL A317  
**Oxygen Vacancies in Oxides Studied by Annihilation of Mono-Energetic Positrons** — •CHRISTOPH HUGENSCHMIDT<sup>1,2</sup>, PHILIP PIKART<sup>1,2</sup>, and KLAUS SCHRECKENBACH<sup>2</sup> — <sup>1</sup>ZWE FRM II, Technische Universität München, Lichtenbergstrasse 1, 85747 Garching — <sup>2</sup>Physik-Department E21, Technische Universität München, James-Franck-Strasse, 85748 Garching

Oxygen vacancies play a fundamental role for the material properties of various oxides, e.g. charge carrier density in high-T<sub>c</sub> superconductors, magnetic properties of diluted magnetic semiconductors or paramagnetic properties of SiO<sub>2</sub>. In this study, open volume defects in (metal) oxides are investigated by Doppler-broadening spectroscopy (DBS) of the positron annihilation. More detailed information about the chemical surrounding at the positron annihilation site is gained by additional coincident DBS experiments, where a signature of positrons annihilating with electrons from oxygen is observed. The mono-energetic positron beam at NEPOMUC [1] was used which allows depth dependent measurements, and hence the investigation of thin oxide layers. Recent results for metallic oxides such as ZnO are presented and compared with various non-metallic oxides such as amorphous and crystalline SiO<sub>2</sub>, oxygen terminated Si-surface, and ice. The role of neutral and charged oxygen vacancies and the application of the positron annihilation technique to study oxygen vacancies will be discussed.

[1] C. Hugenschmidt B. Löwe, J. Mayer, C. Piochacz, P. Pikart, R. Repper, M. Stadlbauer, K. Schreckenbach; Nucl. Instr. Meth. A 593 (2008) 616

DF 2.3 Mon 11:20 WIL A317  
**Electronic properties of defects in SrTiO<sub>3</sub> - theory and experiments** — •TORSTEN WEISSBACH<sup>1</sup>, THOMAS RIEDL<sup>2</sup>, THOMAS GEMMING<sup>2</sup>, SIBYLLE GEMMING<sup>3</sup>, MATTHIAS ZSCHORNAK<sup>1</sup>, EMANUEL GUTMANN<sup>1</sup>, HARTMUT STÖCKER<sup>1</sup>, TILMANN LEISEGANG<sup>1</sup>, and DIRK C. MEYER<sup>1</sup> — <sup>1</sup>Institut für Strukturphysik, TU Dresden — <sup>2</sup>Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden — <sup>3</sup>Forschungszentrum Dresden-Rossendorf

SrTiO<sub>3</sub> is a commercially available wafer material e.g. for the integration of oxide superconductors or microwave filter applications. The electric properties of SrTiO<sub>3</sub> are routinely modified by doping with additional elements such as Nb. A targeted defect engineering may,

however, achieve similar or superior results, while remaining in the ternary system (Sr,Ti,O), i.e. without the need for extrinsic doping. Material characterization methods able to distinguish such defects in particular are needed. In the present study we combine all-electron first-principles calculations with electron energy loss and X-ray absorption spectroscopy to study the electronic properties of SrTiO<sub>3</sub>-related oxygen deficient compounds. In particular, such changes of the SrTiO<sub>3</sub> core-level spectra are studied, which occur if O vacancies accumulate in SrTiO<sub>(3-δ)</sub>, or if excess SrO(001) planes are inserted to form Ruddlesden-Popper-type compounds.

DF 2.4 Mon 11:40 WIL A317

**Spatial Resolution in Electron Energy-Loss Spectroscopy** — ●RALF HAMBACH<sup>1,2</sup>, CHRISTINE GIORGETTI<sup>1,2</sup>, FRANCESCO SOTTILE<sup>1,2</sup>, and LUCIA REINING<sup>1,2</sup> — <sup>1</sup>Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA/DSM, Palaiseau, France — <sup>2</sup>European Theoretical Spectroscopy Facility (ETSF)

The combination of electron energy-loss measurements (EELS) and corresponding *ab initio* calculations has been very productive for the study of collective electronic excitations (plasmons) in solids and nano objects. While most of these investigations have been angular resolved, new techniques allow for atomic spatial resolution (e.g. the UltraSTEM microscope at the LPS, Orsay, France) and call for corresponding theoretical investigations.

First, we have studied the spatial distribution of excitations (plasmons) in Carbon systems using *ab initio* calculations [1] within the framework of time-dependent density functional theory (TDDFT). Second, we present an approach to study spatially resolved EELS in the low loss region (less than 40 eV), explicitly taking into account for non-local effects of the dielectric function.

[1] DP-code: <http://www.dp-code.org>; V.Olevano *et.al.*, unpublished.

DF 2.5 Mon 12:00 WIL A317

**Investigation of the surface charge density of lithium niobate crystals with scanning force microscopy\*** — ●FLORIAN JOHANN, TOBIAS JUNGK, AKOS HOFFMANN, and ELISABETH SOERGEL — Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany

Theoretical calculations of the surface charge density of lithium niobate yield a result of 0.7 C/m<sup>2</sup> for the z-face. It is safe to say that this value can not be true for a real crystal, since this charge density would be high enough to ionize air at a domain boundary. Therefore the real surface charge must be reduced by internal and external compensation mechanisms. The scanning force microscope is a perfect tool to investigate the dependance of the surface charges with respect to temperature, illumination, and humidity. In the end it should be possible to determine an order of magnitude for the really occurring charge density.

\*Financial support from the Deutsche Telekom AG is gratefully acknowledged.

DF 2.6 Mon 12:20 WIL A317

### DF 3: Focus Session: Interactions of Molecules with Dielectric Surfaces

Time: Monday 14:30–17:20

Location: WIL A317

#### Invited Talk

DF 3.1 Mon 14:30 WIL A317

**Interaction of molecules with dielectric surfaces: From single molecular adsorption to functional devices** — ●LUKAS M. ENG — TU Dresden, Institut für Angewandte Photophysik, 01062 Dresden

Heterojunctions formed between organic/biological molecules and dielectric/ferroelectric substrates (such as organic FETs [1]) gain rapidly in interest due to the possibility of inducing novel and tunable functionality on the atomic/molecular scale. We report here on high-resolution topographic and surface potential investigations of polar and non-polar organic molecules deposited onto ultrathin dielectric layers of just 1 monolayer in thickness. Dipole formation was measured for several types of molecules resulting in both donor and acceptor-like molecular behavior for different molecule-substrate interactions [2,3]. Our multi-scale modeling [4] of molecular ordering [5] revealed a strong dependence on local electric fields, leading to distinctly different molecular pattern formation for instance at step edges and defect sites [6]. As such a "defect", we purposely introduced ferroelectric thin films

**k-space spectroscopy on calcium barium niobate single crystals** — ●URS HEINE<sup>1</sup>, UWE VÖLKER<sup>1</sup>, KLAUS BETZLER<sup>1</sup>, MANFRED BURIANEK<sup>2</sup>, and MANFRED MUEHLBERG<sup>2</sup> — <sup>1</sup>Department of Physics, University of Osnabrueck, D-49069 Osnabrueck — <sup>2</sup>Institute of Crystallography, University of Cologne, D-50674 Cologne

We report on domain size distributions in the uniaxial ferroelectric tungsten bronze type calcium barium niobate (CBN). Using non-collinear quasi-phase matched second harmonic generation (*k-space spectroscopy*), we are able to monitor size-dependent changes in the ferroelectric domain structure of the sample under external electric fields and in the vicinity of the ferroelectric phase transition. [001]-oriented transparent and colorless single crystals were grown by the Czochralski method with dimensions of 12 mm in diameter and about 80 mm in length. With its relatively high Curie temperature of about 538 K for 28.1 mole % calcium and its high nonlinear coefficients, CBN is a promising material for future applications. Thus, a detailed knowledge of ferroelectric properties is desirable. Our results reveal a qualitatively similar behaviour compared to the previously investigated relaxor ferroelectric SBN. The domain characteristics during polarization switching and the decay of large domain structures in the vicinity of the phase transition are clearly detectable. Directing the fundamental light beam parallel to the crystallographic c-axis leads to a characteristic cone of second harmonic light which also has been observed in SBN before. The properties of this cone, depending on the poling state of the crystal, have also been investigated.

DF 2.7 Mon 12:40 WIL A317

**Characterization of guanidiniocarbonyl pyrroles in water by pH-dependent UV Raman spectroscopy and component analysis** — SUNIL KUMAR SRIVASTAVA<sup>1</sup>, ●STEPHAN NIEBLING<sup>1</sup>, BERND KÜSTNER<sup>1</sup>, PETER RICHARD WICH<sup>2</sup>, CARSTEN SCHMUCK<sup>2</sup>, and SEBASTIAN SCHLÜCKER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück. — <sup>2</sup>Institut für Organische Chemie, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen.

Guanidiniocarbonyl pyrroles are artificial receptors for the efficient complexation of peptides even in polar solvents such as water. Their carboxylate binding site (CBS) can be probed selectively by ultraviolet resonance Raman (UVRR) scattering. We present a pH-dependent UVRR spectroscopic investigation of two guanidiniocarbonyl pyrroles in water: the model receptor CBS-NH<sub>2</sub> and the peptide receptor CBS-Lys-Lys-Phe-NH<sub>2</sub>. UVRR spectra with 275 nm laser excitation were recorded between pH 6 and pH 7. Within this small pH range near the pK<sub>a</sub> of 6.4, protonated and neutral CBS species are simultaneously present in an acid/base equilibrium. By using non-negative matrix factorization (NMF), the individual UVRR component spectra of these distinct CBS species were determined without any *a priori* knowledge. The pH-dependent UVRR spectra of the small model receptor CBS-NH<sub>2</sub> and the larger peptide receptor CBS-Lys-Lys-Phe-NH<sub>2</sub> can both be described as linear combinations of only two components. Control experiments at pH 2 and pH 10 show an excellent agreement with the derived NMF component spectra and confirm their assignment to the protonated and neutral CBS species, respectively.

having a remnant but switchable surface charge, in order to investigate their applicability as functional gate electrodes in ferroelectric organic field effect transistors. Moreover, we use such ferroelectric templates as templates for the controlled molecular adsorption, as will be demonstrated for nanowires attached along domain walls. - Acknowledgement: DFG. [1] K. Haubner, pss A 205 (2008) 430. [2] P. Milde, NT 19 (2008) 305501-1. [3] U. Zerweck, NT 18 (2007) 084006. [4] S. Gemming, J. Comput.-Aided Mater. Des. 14(S1) (2008) 211. [5] S. Gemming, EPJ: Special Topics 149 (2007) 145. [6] C. Loppacher, NT 17 (2006) 1568.

#### 5 min. break

#### Topical Talk

DF 3.2 Mon 15:05 WIL A317

**Studying terephthalic acid on dielectric surfaces using non-contact atomic force microscopy** — ●PHILIPP RAHE, MARKUS NIMMIRICH, and ANGELIKA KÜHNLE — Fachbereich Physik, Universität

Osnabrück, Germany

Self-assembly of organic molecules is a promising route to fabricating devices on the nanometer scale. While the interaction of molecules with metallic surfaces has been investigated extensively, dielectric surfaces have been studied rather rarely due to both experimental as well as theoretical challenges. For obtaining real-space information on insulators, atomic force microscopy has been established as this technique is not limited to conducting substrates compared to scanning tunnelling microscopy.

Here, we have studied the adsorption characteristics and self-assembly of terephthalic acid (TPA) on two different substrates, namely titania and calcite, using non-contact atomic force microscopy operated under ultra-high vacuum conditions.

On the (110) surface of rutile titania we observe an ordered ( $2\times 1$ ) structure at coverages of about 1 ML, which we attribute to an upright adsorption geometry of TPA. At lower coverages single molecules are observed. In contrast, on the ( $10\bar{1}4$ ) surface of calcite the molecules are mobile at room temperature at coverages less than a monolayer. Experiments at 115 K reveal stable, well-ordered islands. Upon increasing the coverage to 1 ML, we observe a well-ordered structure, which is stable at room temperature. Comparing these two substrates we can evaluate the influence of the dielectric substrate on molecular self-assembly.

**Topical Talk** DF 3.3 Mon 15:25 WIL A317  
**Theoretical contributions to the characterization of adsorbates at titania surfaces** — ●THOMAS BREDOW — Universität Bonn, Institut für Physikalische und Theoretische Chemie, Bonn

Titania is one of the most important materials for heterogeneous catalysis, either as active compound or as support. Despite the large amount of theoretical work that has been correspondingly spent on this subject, several issues concerning surface structure, bonding of adsorbates, and catalytic reaction mechanisms at the titania surfaces, have only recently been addressed.

In this contribution a brief overview of quantum-chemical investigations of titania is presented. Starting from basic properties such as relaxation and energy of low-index rutile and anatase surfaces and electronic effects of simple adsorbates, e.g. metal atoms and dimers, models are presented that take into account solvent effects of titania nanoparticles in aqueous solution, and allow for a spectroscopic characterization of adsorbed species.

**Topical Talk** DF 3.4 Mon 15:45 WIL A317  
**Accurate Energetics of Ground and Excited States of Molecules on Surfaces** — ●THORSTEN KLÜNER — Universität Oldenburg, Theoretische Chemie, 26111 Oldenburg

Photodesorption of small molecules from surfaces is one of the most fundamental processes in surface photochemistry. Despite its apparent simplicity, a microscopic understanding beyond a qualitative picture still poses a true challenge for theory. While the dynamics of nuclear motion can be treated on various levels of sophistication, all approaches suffer from the lack of sufficiently accurate potential energy surfaces, in particular for electronically excited states involved in the desorption scenario.

In the last decade, we have developed a systematic and accurate methodology to reliably calculate accurate ground and excited state potential energy surfaces (PES) for different adsorbate-substrate systems. These potential energy surfaces serve as a prerequisite for subsequent quantum dynamical wave packet calculations, which allow for a direct simulation of experimentally observable quantities such as velocity distributions.

In this contribution, I will focus on recent results obtained for photodesorption of NO and CO from a NiO(100) surface. In contrast to previous studies, we were able to construct highly accurate potential energy surfaces based on correlated quantum chemical calculations (CASPT-2/CCSD(T)). These potential energy surfaces were used in subsequent wave packet studies which reveal new desorption mechanisms. All results are in good agreement with recent experiments.

5 min. break

**Invited Talk** DF 3.5 Mon 16:10 WIL A317  
**Fluorescence and ordering of aromatic molecules on thin dielectric films** — ●MORITZ SOKOLOWSKI — Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

The fluorescence of organic molecules adsorbed on well-defined surfaces constitutes an interesting and powerful probe that completes surface science experiments. In particular, the interplay of structural order and the resulting optical properties due to the intermolecular dipole-dipole coupling is of interest and offers new possibilities to tune the emitting properties. Among the substrate materials, thin epitaxial films of wide-band gap materials are most interesting, since they allow parallel investigations by electron based surface techniques, e.g., low energy electron diffraction or STM, but avoid the ultrafast fluorescence quenching that is otherwise present on metal surfaces. In this talk, the present status of fluorescence experiments on different dielectric thin film (e.g., NaCl,  $\text{AlO}_x$ ) will be reported.

**Topical Talk** DF 3.6 Mon 16:40 WIL A317  
**Determination of Molecule Orientation on Oxide Surfaces by Near-Edge X-ray Absorption Spectroscopy** — ●ALEXEI NEFEDOV, MIKHAIL NABOKA, and CHRISTOF WÖLL — Ruhr Universität Bochum, Germany

Recently, the formation of molecular networks on metals has attracted considerable attention [1]. When replacing the supporting metals by their oxides the situation becomes more complex because the interaction with the ionic centers on the substrate will compete with the molecule-molecule interaction. Since most techniques employed to study adsorption on metals are difficult to apply to oxides because of the insulating nature of these substrates only few works focusing on such systems have been reported so far. Recently, Tekiel et al. [2] studied the adsorption of TPA on  $\text{TiO}_2(110)$  and an upright orientation was reported, which is incompatible with the formation of a two-dimensional network. We have carried out a systematic investigation on the orientation of the TPA-molecules on a rutile  $\text{TiO}_2(110)$  substrate using near-edge x-ray absorption spectroscopy. We have investigated a series of coverages, extending from a few percent of monolayer to saturation corresponding to 1 ML. We find a planar adsorption geometry of TPA molecules up to  $\sim 0.3$  ML, while when saturation coverage is reached the TPA molecules are adsorbed in an upright position. The latter adsorption geometry implies that one of the carboxyl groups binds to the surface as a bidentate carboxylate.

[1] S. Stepanow et al, J. Phys. Chem. B, 108, 19392, (2004).

[2] A. Tekiel et al, J. Phys. Chem. C, 112, 12606, (2008).

**Topical Talk** DF 3.7 Mon 17:00 WIL A317  
**Adsorption of Organic Molecules on Moderately Reactive Substrates** — ●MICHAEL ROHLFING<sup>1</sup>, ANDREAS GREULING<sup>1</sup>, and THOMAS BREDOW<sup>2</sup> — <sup>1</sup>Fachbereich Physik, Universität Osnabrück, Germany — <sup>2</sup>Institute for Physical and Theoretical Chemistry, Universität Bonn, Germany

We discuss the adsorption of organic molecules on crystal surfaces within density-functional theory (DFT), focusing on three examples of moderate molecule-substrate interaction. PTCDI, which is a flat elongated molecule, binds to rutile  $\text{TiO}_2(110)$  in a flat-lying configuration with orientation along the rows, showing high mobility along the rows. TMA, on the other hand, interacts with rutile  $\text{TiO}_2(110)$  via COOH groups at preferred sites, resulting in specific, flat-lying configurations. Thirdly, PTCDA adsorbs on Ag(111) by delocalized interaction of its perylene core plus local binding via its oxygen corner groups. All results are discussed in context with available experimental data.

Our studies demonstrate very different relaxation time scales of intramolecular and molecule-substrate coordinates, driven by the much different respective energies. This requires particular care in all optimization procedures. Furthermore, we discuss the validity of various exchange-correlation functionals, in comparison with more advanced adsorption energies from an exact-exchange-and-correlation (EXX+RPA) formalism. Our EXX+RPA and DFT results for PTCDA/Ag(111) demonstrate that the most reliable DFT data are obtained from the local-density approximation (LDA), which we use throughout our DFT studies, therefore.

## DF 4: Multiferroics, Phase Transitions &amp; Relaxors

Time: Monday 10:00–12:40

Location: WIL B321

## Invited Talk

DF 4.1 Mon 10:00 WIL B321

**Magnetoelectric effects and excitations in multiferroic manganites** — ●ANDREI PIMENOV — Experimentelle Physik 4, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Multiferroics are materials simultaneously showing ferromagnetic and ferroelectric order. Two order parameters are coupled in these materials, which leads to such unusual effects like magnetic switching of electric polarization and dielectric constant. As can be expected already from the first principles, changes in the static properties of multiferroics must be accompanied by dynamic effects like characteristic magnetoelectric excitations. Indeed, such excitations could be recently observed in the spectra and were called electromagnons. Contrary to the conventional magnons, the electromagnons are excited by the electric component of the electromagnetic wave and contribute to the static dielectric permittivity. The suppression of electromagnons in external magnetic fields provides a natural explanation for the magnetoelectric effects in broad frequency range between dc and terahertz.

## 5 min. break

DF 4.2 Mon 10:40 WIL B321

**Multiglassy systems based on incipient ferroelectrics** — ●VLADIMIR SHVARTSMAN<sup>1</sup>, PAVEL BORISOV<sup>1</sup>, SUBHANKAR BEDANTA<sup>1</sup>, ALEKSANDER TKACH<sup>2</sup>, PAULA VILARINHO<sup>2</sup>, and WOLFGANG KLEEMANN<sup>1</sup> — <sup>1</sup>Angewandte Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — <sup>2</sup>Department of Ceramics and Glass Engineering, CICECO, University of Aveiro, 3810-193, Aveiro, Portugal

In recent years there has been growing scientific interest in materials exhibiting the magnetoelectric (ME) effect. Research has mainly been focused on multiferroic materials, where two or more ferroically ordered states exist simultaneously. We show that the class of ME materials may be extended to those, where two glassy states of different nature occur simultaneously. This can be realized in incipient ferroelectrics like SrTiO<sub>3</sub> or KTaO<sub>3</sub> moderately doped with a paramagnetic cation, e.g. with Mn<sup>2+</sup> [1]. The transitions into glassy states manifest themselves by anomalies in the temperature dependencies of the dielectric and magnetic susceptibilities as well as by a particular memory effects ("hole burning"). The ME effects were directly measured using a modified SQUID susceptometer. Although the amount of magnetically active ions is relatively small, a strong higher order ME coupling via both the "paramagnetoelectric" EH<sup>2</sup> and the "magneto-capacitive" E<sup>2</sup>H<sup>2</sup> effects is observed.

[1] V.V. Shvartsman, S. Bedanta, P. Borisov, W. Kleemann, A. Tkach, P.M. Vilarinho, Phys. Rev. Lett. 101 (2008) 165704.

DF 4.3 Mon 11:00 WIL B321

**Dimensional crossover and absence of quantum criticality in SrTi<sup>16</sup>O<sub>1-x</sub><sup>18</sup>O<sub>x</sub>** — ●ANNETTE BUSSMANN-HOLDER<sup>1</sup> and ALAN R. BISHOP<sup>2</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart — <sup>2</sup>Los Alamos National Laboratory, Theoretical Division, Los Alamos NM887545, USA

The isotope-induced ferroelectricity observed in SrTi<sup>18</sup>O<sub>3</sub> (STO18) enables a systematic study of the crossover between quantum paraelectricity and ferroelectricity as a function of x in SrTi<sup>16</sup>O<sub>1-x</sub><sup>18</sup>O<sub>x</sub> (STO16<sub>1-x</sub>STO18<sub>x</sub>). We predict that all ferroelectric compounds have a finite transition temperature T<sub>c</sub> and show a dimensionality crossover from d=3 to d=4 at sufficiently low temperature. A discontinuity in behavior takes place around x=0.35, where quantum fluctuations suppress the transition. No evidence is found for a quantum critical point in the phase diagram. The high temperature structural transition shows a substantial isotope dependence which is, however, less striking than for the ferroelectric transition.

DF 4.4 Mon 11:20 WIL B321

**Effect of Ru doping on the structure and properties of PbZn<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub>-PbTiO<sub>3</sub> near the morphotropic phase boundary** — TORBEN SCHOLZ<sup>1</sup>, ●BORIANA MIHAILOVA<sup>2</sup>, GEROLD A. SCHNEIDER<sup>1</sup>, NILS PAGELS<sup>3</sup>, JÜRGEN HECK<sup>3</sup>, MARIN GOSPODINOV<sup>4</sup>, and ULRICH BISMAYER<sup>2</sup> — <sup>1</sup>Institute of Advanced Ceramics, Hamburg University of Technology — <sup>2</sup>Institute of Mineralogy and Petrology, University of Hamburg — <sup>3</sup>Institute of Inorganic and Applied Chem-

istry, University of Hamburg — <sup>4</sup>Institute of Solid State Physics, Bulgarian Academy of Sciences

The search for novel multifunctional materials has spotted Pb-based perovskite-type solid solutions of relaxor and normal ferroelectrics because of their huge electromechanical coupling and strong photoelastic effects near the morphotropic phase boundary. We studied the local atomic structure, domain pattern and properties of pure and Ru-doped 0.9PbZn<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub>-0.1PbTiO<sub>3</sub> single crystals by applying atomic and piezoresponse force microscopy (AFM/PFM), dielectric measurements, X-ray diffraction analysis, Raman scattering and electron paramagnetic resonance. AFM/PFM images reveal the existence of tetragonal and non-tetragonal ferroelectric domains in 0.9PZN-0.1PT. The dielectric and elastoelectric loops show that Ru doping, Ru/(Ti+Zn+Nb) = 0.002, leads to significant ferroelectric hardening due to the immobilization of domain walls. Besides, the addition of Ru decreases the ferroelectric domain size, reduces the polar fraction distributed in the pseudo cubic matrix and changes the unit cell parameters of the overall tetragonal structure.

DF 4.5 Mon 11:40 WIL B321

**Ferroelectric Domains Nucleation and Growth in BaTiO<sub>3</sub>** — ●STEFANO LEONI<sup>1</sup>, MAREK PASCIAK<sup>2</sup>, and SALAH EDDINE BOULFELFEL<sup>1</sup> — <sup>1</sup>Max-Planck-Institut CPFS, Dresden, Germany — <sup>2</sup>Institute of Low Temperature, PAS, Wroclaw, Polen

Ferroelectric materials are broadly employed as capacitors and memory materials. However, even for the classical compound BaTiO<sub>3</sub> (BTO), the microscopic nature of the cubic paraelectric (PE) and of the ferroelectric (FE) phases and phase transformations (from cubic to tetragonal, orthorhombic and rhombohedral phases on lowering temperature) is still unclear. However, a deep understanding of the phenomenon of ferroelectricity is of top priority for further material properties control. We perform molecular dynamics simulations based on advanced schemes on the PE to FE phase transition in BTO. We elucidate ferroelectric domain nucleation and growth in detail, stressing the role of anti-ferroelectric coupling in FE domains, and show how a rescaling of critical lengths is accompanying the transition and is responsible for the ferroelectric response of the material. A full picture of domain formation with and without an external field is presented.

DF 4.6 Mon 12:00 WIL B321

**Pressure-induced local structural changes in PSN, PSN:Ba and PSN:Bi** — ●ANNA-MARIA WELSCH<sup>1</sup>, BORIANA MIHAILOVA<sup>1</sup>, MARIN GOSPODINOV<sup>2</sup>, RAINER STOSCH<sup>3</sup>, BERND GUETTLER<sup>3</sup>, and ULRICH BISMAYER<sup>1</sup> — <sup>1</sup>Universität Hamburg — <sup>2</sup>Bulgarian Academy of Sciences — <sup>3</sup>PTB Braunschweig

Relaxors represent a special class of ferroelectrics which are attractive for a number of technological applications due to their unusual dielectric properties, intimately related to the presence of polar nanodomains within paraelectric matrix. Majority of relaxors are of Pb-based perovskite-type structure with general formula being ABO<sub>3</sub>, which enables substitutional disorder in both A- and B-sites. Different types of cations on A- and B- positions and their degree of order have a direct influence on the formation and behaviour of polar nanodomains. In the recent years pressure came forth as a very powerful experimental approach in investigating the origin and true mechanism of relaxor behaviour, both still elusive to this day in spite of years of extensive research. Pressure acts directly on the inter-atomic level and combined with variations in the chemical composition influence the nano-domain structure and desired relaxor properties.

Here we present our results on the structure of pure, Ba- and Bi-containing PbSc<sub>0.5</sub>Nb<sub>0.5</sub>O<sub>3</sub>. The pressure-induced structural changes of differently A-site doped compounds were studied by Raman spectroscopy. Our results indicate that pressure induces structural changes, favouring a certain type of ferroic distortion, with varying degree relative to the type and stereochemical nature of the A-site cations.

DF 4.7 Mon 12:20 WIL B321

**Niobate (PSN) and A-site Doped PSN at High Pressures** — ●BERND MAIER<sup>1</sup>, CARSTEN PAULMANN<sup>1</sup>, ROSS ANGEL<sup>2</sup>, JENS ENGEL<sup>3</sup>, MARTIN GOSPODINOV<sup>4</sup>, BORIANA MIHAILOVA<sup>1</sup>, and ULRICH BISMAYER<sup>1</sup> — <sup>1</sup>Mineralogisch-Petrographisches Institut, Universität Hamburg —

<sup>2</sup>Crystallography Laboratory, Virginia Tech, Blacksburg, USA —  
<sup>3</sup>Institut für Werkstoffwissenschaften, Technische Universität Dresden —  
<sup>4</sup>Institute of Solid State Physics, Bulgarian Academy of Sciences, Sofia, Bulgaria

High-pressure single crystal X-ray diffraction studies at room temperature on the relaxor ferroelectric lead scandium niobate (PSN) as well as Ba- and Bi-doped PSN are presented. A change in the volume compressibility, broadening of diffraction peaks, suppression of diffuse scattering, and the appearance of (hkl)-reflections ( $h, k, l = 2n+1$ ) using the  $Fm\bar{3}m$ -cell shows that PSN undergoes a phase transition near

2 GPa which is consistent with the results of M. Somayazulu [1]. For A-site doped PSN, the phase transition occurs at around 3.5 GPa. The transition for Bi-doped PSN is better pronounced than that for Ba-doped PSN. The suppression of the diffuse scattering at pressures above the phase transition is associated with a decoupling of A- and B-site cations in the existing polar nanoregions which leads to an enhancement of the ferroic distortion in the PbO-system. The decoupling also allows the B-site cations to shift back from their off-center positions which leads to the appearance of the reflections in the (hkl)-layers ( $l = 2n+1$ ).

[1] Somayazulu, M. et al., APS Meeting Abstracts (2008)

## DF 5: High-k and low-k Dielectrics

Time: Monday 15:00–17:00

Location: WIL B321

DF 5.1 Mon 15:00 WIL B321

**Dielectric properties of  $A_{2/3}Cu_3Ti_4O_{12}$  ( $A = La, Pr, Nd, Sm, Eu, Gd, Tb, Dy$ )** — ●JÜRGEN SEBALD<sup>1</sup>, STEPHAN KROHNS<sup>1</sup>, PETER LUNKENHEIMER<sup>1</sup>, STEFAN RIEGG<sup>2</sup>, STEFAN G. EBBINGHAUS<sup>3</sup>, and ALOIS LOIDL<sup>1</sup> — <sup>1</sup>Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Solid State Chemistry, University of Augsburg, 86135 Augsburg, Germany — <sup>3</sup>Institute for Chemistry, Martin-Luther University Halle-Wittenberg, 06120 Halle, Germany

New materials showing the phenomenon of a very high dielectric constant ( $\epsilon' > 10^3$ ), similar to the famous  $CaCu_3Ti_4O_{12}$  (CCTO), are in the focus of scientific interest. Materials with extremely high ("colossal") dielectric constants (CDC) are urgently needed for future electronics. Today it is more or less commonly accepted that the CDC is due to extrinsic effects like "internal barrier layer capacitors" (IBLC) or "surface barrier layer capacitors" (SBLC). Polarisation effects at grain boundaries or other internal barriers can generate nonintrinsic colossal values of  $\epsilon'$  (IBLC). In addition, SBLCs, arising, e.g., from a formation of Schottky diodes at the contact-bulk interfaces, can generate a contribution to the colossal value of  $\epsilon'$  as has been shown for  $CaCu_3Ti_4O_{12}$ . To investigate these models and to search for alternatives for CCTO, frequency- and temperature-dependent dielectric measurements on differently treated samples of various CCTO related materials were performed. To check for possible correlations of magnetic structure and dielectric properties, magnetic-field dependent dielectric spectroscopy was carried out.

DF 5.2 Mon 15:20 WIL B321

**Characterization of  $(SrO)_x(ZrO_2)_{(1-x)}$  thin films for use in metal insulator metal capacitors** — ●MATTHIAS GRUBE<sup>1</sup>, OLIVER BIERWAGEN<sup>2</sup>, DOMINIK MARTIN<sup>1</sup>, LUTZ GEELHAAR<sup>3</sup>, and HENNING RIECHERT<sup>3</sup> — <sup>1</sup>NamLab GmbH, 01187 Dresden — <sup>2</sup>University of California, Santa Barbara 93106 CA, USA — <sup>3</sup>Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin

$(SrO)_x(ZrO_2)_{(1-x)}$  is a promising candidate as high-k dielectric for metal-insulator-metal capacitors of future memory cells. The dielectrics were grown by co-evaporating SrO from a high temperature effusion cell and ZrO<sub>2</sub> from an electron beam evaporator in a molecular beam deposition chamber. As substrates, n<sup>++</sup>-Si-wafers were used that were covered with a pre-deposited 5 nm-thin TiN layer. In order to reveal the correlation between process conditions and film properties, especially high-k values and leakage currents, a series of samples with different thicknesses ranging from 10 to 40 nm were fabricated while the growth temperature was varied from 100°C to 800°C. X-ray fluorescence analysis (XFA) and X-ray reflectometry (XRR) were employed to determine the thickness and the stoichiometry of the films, while the electrical properties of the dielectrics were determined through current-voltage and capacitance-voltage measurements before and after a post deposition anneal.

DF 5.3 Mon 15:40 WIL B321

**Ternary rare-earth based alternative gate-dielectrics for future integration in MOSFETs** — ●JÜRGEN SCHUBERT, JOAO MARCELO LOPES, EYLEM DURGUN ÖZBEN, ROMAN LUPTAK, STEFFI LENK, WILLI ZANDER, and MARTIN ROECKERATH — IBN 1-IT, Forschungszentrum Jülich, 52425 Jülich

The dielectric SiO<sub>2</sub> has been the key to the tremendous improvements in Si-based metal-oxide-semiconductor (MOS) device performance over

the past four decades. It has, however, reached its limit in terms of scaling since it exhibits a leakage current density higher than 1 A/cm<sup>2</sup> and does not retain its intrinsic physical properties at thicknesses below 1.5 nm [1,2]. In order to overcome these problems and keep Moore's law ongoing, the use of higher dielectric constant (k) gate oxides has been suggested. These high-k materials must satisfy numerous requirements such as the high k, low leakage currents, suitable band gap and offsets to silicon. Rare-earth based dielectrics are promising materials which fulfill these needs. We will review the properties of RE<sub>2</sub>ScO<sub>3</sub> (RE = La, Dy, Gd, Sm, Tb) and LaLuO<sub>3</sub> thin films, grown with pulsed laser deposition, e-gun evaporation or molecular beam deposition, integrated in capacitors and transistors. A k > 20 for the RE<sub>2</sub>ScO<sub>3</sub> (RE = Dy, Gd) and around 30 for (RE = La, Sm, Tb) and LaLuO<sub>3</sub> are obtained. Transistors prepared on SOI and sSOI show mobility values up to 380 cm<sup>2</sup>/Vs on sSOI, which are comparable to such prepared with HfO<sub>2</sub>. [1] X. Gou, and T. P. Ma, IEEE Electron Device Lett. 19, 207 (1998). [2] D. A. Muller, T. Sorsch, S. Moccio, F. H. Baumann, K. Evans-Lutterodt, and G. Timp Nature 399, 758 (1999).

DF 5.4 Mon 16:00 WIL B321

**The deposition of rare-earth oxide ultrathin-films with inorganic precursors** — ●MARAIKE AHLF<sup>1</sup>, HANNO SCHNARS<sup>1</sup>, OLIVER SKIBITZKI<sup>1</sup>, MARVIN ZÖLLNER<sup>1</sup>, KATHARINA AL-SHAMERY<sup>1</sup>, MAREIKE AHLERS<sup>2</sup>, and MATHIAS WICKLEDER<sup>2</sup> — <sup>1</sup>University of Oldenburg, Institute for Pure and Applied Chemistry, Physical Chemistry I — <sup>2</sup>University of Oldenburg, Institute for Pure and Applied Chemistry, Inorganic Chemistry

Semiconductor industry is searching for new materials as gate-oxides in MOSFETs (Metal Oxide Semiconductor Field Effect Transistors) because the goal to shrink the size is limited due to the quantum mechanical tunnelling of electrons through a very thin oxide layer. Therefore it is necessary to replace the conventionally used gate-oxide material SiO<sub>2</sub> by new materials with higher  $\kappa$ -value and a bigger band gap, which could be rare-earth oxides (REO's) e.g. To prevent interfacial layers of SiO<sub>2</sub> in our investigation, the Si-wafers are prepared by a wet chemical etching using HF and NH<sub>4</sub>F before depositing new RE-based inorganic precursors. The mechanism of decomposition of RE-nitrates is studied in UHV by using STM, XPS and TPD. The used precursors are expected to decompose carbonfree to form the REO and gaseous decomposition products under mild, sputter free heating conditions. Deposition is done by using a liquid injection doser, drop-cast and dip applying different organic solvents. SEM and HRTEM images are utilized to assess the effectiveness of the different deposition conditions to form uniform, defectfree REO-ultrathin-films on Si with filmthickness of less than 10 nm state of the art related to our research.

DF 5.5 Mon 16:20 WIL B321

**High performance MIM capacitors with Atomic Vapour Deposited HfO<sub>2</sub> dielectrics** — ●MINDAUGAS LUKOSIUS, CHRISTIAN WENGER, CHRISTIAN WALCZYK, and HANS-JOACHIM MÜSSIG — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Metal-Insulator-Metal (MIM) capacitors are widely used in ICs for Radio-Frequency (RF) applications. Currently, capacitors fabricated by performing MIM structures use silicon oxide or silicon nitride as an insulating layer. However the capacitance density of these materials is limited by low dielectric constant values. Therefore, for further integration of passive components such as capacitors into CMOS devices, dielectric materials with higher permittivity than SiO<sub>2</sub> ( $k =$

3.9) are required. Using the high dielectric constant (high-k) material  $\text{HfO}_2$  as a dielectric in MIM capacitor seems to be a very promising approach. Atomic Vapour Deposition (AVD\*) technique was used for the preparation of hafnium oxide films on 20nm TiN/2nmSiO<sub>2</sub>/Si (200mm) substrates using  $\text{Hf}(\text{NEtMe})_4$  precursor for MIM applications in back-end of line (BEOL). The influence of process temperature (320 - 425 °C) and process pressure (2-10mbar) on the structural and electrical properties of  $\text{HfO}_2$  were investigated. The optimized dielectric layers obtained at 320 °C and 4 mbar possess k value of 18, capacitance density of 3.5 fF/ $\mu\text{m}^2$  combined with required capacitance voltage linearity (<100 ppm/V<sup>2</sup>) and quality factor of 50. Films with thickness of 35 nm exhibit leakage current density of  $2 \cdot 10^{-7}$  A/cm<sup>2</sup> and breakdown strength of 5.8 MV/cm, therefore AVD\* deposited  $\text{HfO}_2$  layers are possible alternative dielectric candidates for MIM applications.

DF 5.6 Mon 16:40 WIL B321  
**Growth investigation of thin Ti-based high-k films** —  
 ●ANDREAS KRAUSE, DOMINIK MARTIN, MATTHIAS GRUBE, and WALTER M. WEBER — namlab gGmbH, D-01187 Dresden

With the further increase in integration density of microelectronics, ordinary SiO<sub>2</sub>-based stacks reach their limits as leakage currents increase significantly. Therefore, dielectric materials are required that combine a high dielectric constant (k) and low leakage currents, such as Ti-based oxides. Different titanates, like  $\text{HfTiO}_x$  or  $\text{CaTiO}_x$  with thicknesses up to 100 nm were deposited via an UHV sputtering tool. As substrates, n<sup>++</sup>-Si-wafers were used as well as Si-wafers coated with TiN or noble metal (Ru, Pt) layers. The morphology was studied with atomic force microscopy and capacitor-voltage measurements were performed to extract the k-value.

## DF 6: Poster I

Time: Tuesday 9:30–12:30

Location: P5

DF 6.1 Tue 9:30 P5

**Atomic layer deposition and characterization of bismuth oxide thin films** — ●PHILIPP MORITZ LEUFKE<sup>1</sup>, NICOLE DONIA<sup>2</sup>, SANJAY MATHUR<sup>3</sup>, and HORST HAHN<sup>1</sup> — <sup>1</sup>Institute of Nanotechnology, Karlsruhe Research Centre, D-76344 Eggenstein-Leopoldshafen, Germany — <sup>2</sup>Leibniz-Institute for New Materials, D-66123 Saarbruecken, Germany — <sup>3</sup>University of Cologne, Institute of Inorganic Chemistry, D-50939 Cologne, Germany

We report on the deposition of thin films of bismuth oxide by atomic layer deposition (ALD). We used bismuth *tert*-butoxide [ $\text{Bi}(\text{OtBu})_3$ ] [1] as a bismuth precursor for the first time. H<sub>2</sub>O serves as oxidizing precursor. Our aim was to overcome the problems caused by known precursors for bismuth containing oxides, which are often thermally unstable and require liquid-injection techniques or do not decompose entirely, leaving impurities in the resulting film [2].

Surface morphology and crystal structure of the prepared thin films are investigated by means of scanning electron microscopy and X-ray diffraction. Energy-dispersive X-ray spectroscopy and X-ray Photoelectron Spectroscopy are employed for chemical analysis. In our studies we show that the morphology depends on various substrates and deposition parameters in these thin films.

[1] M. Mehring, *Coordination Chemistry Reviews, 19th Main Group Chemistry* **251**, 974-1006 (2007)

[2] M. Vehkamäki *et al.*, *Journal of Materials Chemistry* **14**, 3191-3197 (2004)

DF 6.2 Tue 9:30 P5

**Electronic defect state mapping in strontium titanate by surface photovoltage and photoconductivity spectra** — ●JANA BECHERER, ELKE BEYREUTHER, ANDREAS THIESSEN, STEFAN GRAFSTRÖM, and LUKAS M. ENG — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

Within the current interest in the field of oxide electronics, strontium titanate ( $\text{SrTiO}_3$ , STO) plays a crucial role as a substrate for the epitaxy of a wide variety of perovskite oxide films on the one hand and as a functional oxide by itself on the other hand. However, the electronic properties of STO – though having been the subject of research for several decades – are still not well understood for several reasons: (i) Firstly, the electronic properties change dramatically as a function of oxygen content, doping, or surface treatments, while (ii) secondly, standard electrical characterization methods fail due to the wide band gap and the consequently low carrier concentration. Thus optical techniques are the methods of choice for this kind of material.

In order to gain a more systematic understanding of surface and bulk electronic defect states, we performed a comparative study of the spectral, temporal, and temperature dependence of the surface photovoltage and the photoconductivity of undoped and doped STO single crystals. We discuss the defect state distribution within the framework of a classical band scheme.

DF 6.3 Tue 9:30 P5

**Hyperfeinwechselwirkung in dünnen Schichten von  $\text{HfO}_2$**  — ●MICHAEL STEFFENS und REINER VIANDEN — Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn

Der Einsatz von sogenannten "high- $\kappa$ "-Dielektrika als Gate-Oxide in

MOSFET-Strukturen gilt als eine der Möglichkeiten den Miniaturisierungsprozess in der Halbleiter-Industrie voranzutreiben. Als aussichtsreichstes Material wird dabei  $\text{HfO}_2$  angesehen, wobei die thermische Stabilität problematisch bleibt.

In dieser Arbeit wird die Hyperfeinwechselwirkung des Hf in dünnen Schichten  $\text{HfO}_2$  mit der gestörten  $\gamma$ - $\gamma$ -Winkelkorrelation (PAC) untersucht. Die PAC eignet sich besonders für die Bestimmung der lokalen Umgebung eines Sondenkerns im Material. Die PAC-Sonde <sup>181</sup>Hf wird dabei entweder durch Neutronenaktivierung von <sup>180</sup>Hf erzeugt oder direkt in das Material implantiert. Zusätzliche Messungen werden mit der Sonde <sup>111</sup>In durchgeführt.

Die 100 nm bzw. 10 nm dünnen Filmproben sind mit ALCVD und MOCVD auf einem (100) Si-Substrat gewachsen. Im Mittelpunkt der Messungen stehen die Änderungen der Kristallstruktur in der Umgebung der Sonden während eines isochronen Ausheilprogramms und während temperaturabhängigen Messungen, die 'in-situ' stattfinden. Die Ergebnisse der Messungen an diesen dünnen Schichten werden mit Messungen an reinem  $\text{HfO}_2$  verglichen.

DF 6.4 Tue 9:30 P5

**Development of a precisely tuneable continuous-wave THz spectrometer with interferometric frequency control** — ●HOLGER SCHMITZ<sup>1</sup>, JOACHIM HEMBERGER<sup>1</sup>, ANSELM DENINGER<sup>2</sup>, AXEL ROGGENBUCK<sup>2</sup>, and MARKUS GRÜNINGER<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, D-50937 Köln, Germany — <sup>2</sup>TOPTICA Photonics AG, Lochhamer Schlag 19, D-82166 Gräfelfing, Germany

We will report on the development of a precisely tuneable continuous-wave THz spectrometer with interferometric frequency control. The system is based on mixing two near-infrared distributed feedback diode lasers, the beat of which can be tuned continuously from 0 to 1.2 THz. Each laser is stabilized by electronic feedback from a low-finesse Fabry-Perot etalon, yielding a laser linewidth of roughly 1 MHz and a frequency precision of a few MHz. The laser beat is converted into THz radiation by a photoconductive switch, which efficiently generates THz radiation from 20 GHz to 1.2 THz. The THz radiation is detected via a second photoconductive switch via homodyne mixing of the THz signal and the laser beat. The coherent homodyne detection preserves the phase information of the THz electric field, so that both the real and the imaginary part of the dielectric function,  $\epsilon_1$  and  $\epsilon_2$ , can be determined. Making use of different optical path lengths for the laser beam and the THz radiation, the phase shift due to the sample can be determined by sweeping over an interference fringe, typically a few 100 MHz. Thus  $\epsilon_1$  and  $\epsilon_2$  can be determined without mechanically moving parts. First results obtained with this system will be reported.

DF 6.5 Tue 9:30 P5

**The electronic band diagram of thin  $\text{PrO}_2(111)$  / Pr-silicate buffers on Si(111) and its relevance to dielectric properties** — ●OLAF SEIFARTH<sup>1</sup>, CHRISTIAN WALCZYK<sup>1</sup>, GRZEGORZ LUPINA<sup>1</sup>, PETER ZAUMSEIL<sup>1</sup>, DIETER SCHMEISSER<sup>2</sup>, HANS-JOACHIM MÜSSIG<sup>1</sup>, and THOMAS SCHROEDER<sup>1</sup> — <sup>1</sup>IHP, 15236 Frankfurt, Im Technologiepark 25 — <sup>2</sup>BTU Cottbus, 03046 Cottbus, Konrad-Wachsmann Allee 17

Thin dielectric buffers of cubic  $\text{PrO}_2(111)$  on Si(111) are ideally suited to integrate Ge onto Si by moderating the lattice mismatch between the



materials. The leakage current across this dielectric buffer is strongly influenced by the electronic band diagram and defects inside the band gap. Therefore, we measured the band offsets, band gaps and defect positions by means of synchrotron radiation based photoemission spectroscopy techniques (XPS and XAS) with special emphasis on the Pr-silicate interface. In a next step we compare the spectroscopic data with information from dielectric studies, based on temperature dependent leakage current studies. We observe a close relation between dielectric properties and the electronic structure.

DF 6.6 Tue 9:30 P5

**Post deposition annealing induced transition from Pr<sub>2</sub>O<sub>3</sub> to PrO<sub>2</sub> films on Si(111)** — ●THOMAS WEISEMOELLER<sup>1</sup>, FLORIAN BERTRAM<sup>1</sup>, SEBASTIAN GEVERS<sup>1</sup>, ANDREAS GREULING<sup>1</sup>, CARSTEN DEITER<sup>2</sup>, HOLGER TOBERGTE<sup>1</sup>, MANFRED NEUMANN<sup>1</sup>, JOACHIM WOLLSCHLÄGER<sup>1</sup>, ALESSANDRO GIUSSANI<sup>3</sup>, and THOMAS SCHROEDER<sup>3</sup> — <sup>1</sup>Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — <sup>2</sup>HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — <sup>3</sup>Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Films of hexagonal praseodymium sesquioxide (Pr<sub>2</sub>O<sub>3</sub>) were deposited on Si(111) by molecular beam epitaxy and thereafter annealed in oxygen at different temperatures, ranging from 100°C to 700°C. XRR, XRD and GIXRD measurements were performed at beamlines W1 and BW2 at HASYLAB/DESY to analyze the structure of oxide films and interfaces. The films of the samples annealed at 300°C or more were transformed to PrO<sub>2</sub> with B oriented Fm $\bar{3}$ m structure, while films annealed at lower temperatures keep the hexagonal structure. The films compose of coexisting PrO<sub>2</sub> and PrO<sub>2- $\delta$</sub>  species which coexist lateral. The oxygen vacancies are partly ordered lateral and increase the vertical lattice constant of the film, whereas the horizontal lattice constant is almost identical for both species and on all samples. The latter lattice constant matches the lattice constant of the originally crystallized hexagonal praseodymium sesquioxide. That means that no long range reordering of the praseodymium atoms takes place.

DF 6.7 Tue 9:30 P5

**Pulsed laser deposition of praseodymium oxide on silicon at oxygen background** — ●BIWANG YANG, MARKUS RATZKE, and JÜRGEN REIF — LS Experimentalphysik II, BTU Cottbus und IHP/BTU JointLab, Konrad-Wachsmann-Allee 1, D-03046 Cottbus

Praseodymium oxide thin films, as a potential high-k candidate for future silicon microelectronics, can be produced by Pulsed-Laser Deposition (PLD).

However, in contrast to expectation, the procedure does not transfer the stoichiometry of the target material, the films appear to be oxygen deficient. To compensate for this loss of oxygen, the reason of which is not yet clear, we applied an additional oxygen background in our deposition chamber at different pressures.

While both the growth rate and the oxygen content of the layers, produced in this way, show a distinct dependency on oxygen pressure, the electrical properties are not significantly different from films deposited without background gas.

DF 6.8 Tue 9:30 P5

**Structure and Physical Properties of A<sub>2/3</sub>Cu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub> (A = Rare Earth)** — ●STEFAN RIEGG<sup>1</sup>, JÜRGEN SEBALD<sup>3</sup>, STEPHAN KROHNS<sup>3</sup>, STEFAN G. EBBINGHAUS<sup>2</sup>, PETER LUNKENHEIMER<sup>3</sup>, ALOIS LOIDL<sup>3</sup>, and ARMIN RELLER<sup>1</sup> — <sup>1</sup>Solid State Chemistry, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Solid State Chemistry, Institute for Chemistry, Martin-Luther University Halle-Wittenberg, 06120 Halle, Germany — <sup>3</sup>Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Many materials based on the ACu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub> structure-type provide very high dielectric constant  $\epsilon'$ , like the most famous member A = Ca with a value of greater than 10<sup>3</sup>. These materials with so called "colossal dielectric constants" (CDC) are very useful for technical application and thus of special scientific interest. Structurally related systems with lanthanide ions on the A position can be used to study the CDC mechanism. Due to the +3 (Ce: +4) valence of the rare earth ions, in comparison to the +2 valence of Ca, only two thirds (Ce: half) of the A position are occupied in the crystal. Samples with A = Y<sup>3+</sup>, La<sup>3+</sup>, Ce<sup>4+</sup>, Pr<sup>3+</sup>, Nd<sup>3+</sup>, Sm<sup>3+</sup> to Yb<sup>3+</sup> were prepared by solid state reaction of the binary oxides. X-ray diffraction in combination with Rietveld analysis was used to investigate the structure. The measured dielectric properties show the CDC behaviour of this material. In ad-

dition the band gap energy was determined by UV-Vis spectroscopy. Measurements of the magnetic susceptibility were carried out to study the magnetic behaviour.

DF 6.9 Tue 9:30 P5

**Influence of rare earth doping on the phase transition characteristic of strontium barium niobate and a comparison to calcium barium niobate** — ●ALEXANDER NIEMER<sup>1</sup>, URS HEINE<sup>1</sup>, UWE VOELKER<sup>1</sup>, KLAUS BETZLER<sup>1</sup>, and MANFRED MUEHLBERG<sup>2</sup> — <sup>1</sup>University of Osnabrück, Department of Physics, Barbarastr. 7, 49076 Osnabrück — <sup>2</sup>University of Cologne, Institute of Crystallography, Zülpicher Str. 49b, 50674 Cologne

The ferroic relaxor strontium barium niobate (SBN) shows interesting dielectric properties foremost in the region of its smeared phase transition. Here, the influence of rare earth doping on the relaxor characteristic is studied for SBN by analyzing the complex dielectric constant. As dopants, Erbium (0 to 1.04 mol%), Ytterbium (0 to 1.56 mol%), and Europium (0 to 1.14 mol%) were used. As a result the rare earth doping has significant impact on the phase transition behavior, regarding both, temperature and smearing. Since the use of SBN in technical applications is constrained due to the low phase transition temperature, we analyzed the dielectric behavior of the unfilled tungsten bronze calcium barium niobate (CBN). Congruently melting CBN (28.1 mole fraction calcium [1]) exhibits a phase transition at about 540 K, nearly 200 K higher than the one of SBN61. A comparison between the dielectric constant of SBN and CBN yields, that these two materials show a substantially different phase transition behavior, despite the crystal structures show similarities.

[1] M. Burianek, B. Joschko, I. Kerkamm, T. Schoenbeck, D. Klimm, M. Muehlberg: J. Crystal Growth 229, 413-417 (2007)

DF 6.10 Tue 9:30 P5

**Strain and electric field effects on the dielectric permittivity of epitaxial SrTiO<sub>3</sub> thin films** — ●SEBASTIAN ENGMANN, VEIT GROSSE, ROBERT HAEHLE, JANINE FISCHER, and PAUL SEIDEL — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, 07743 Jena

We present measurements of the dielectric permittivity of epitaxial SrTiO<sub>3</sub> (STO) thin films. Therefore we prepared capacitor structures based on the multilayer system YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub>/STO/Au grown by pulsed laser deposition on LaAlO<sub>3</sub> substrates. Rocking curves prove good c-axis orientation of the STO crystallites. Due to epitaxial strain for thin films the c-axis is enlarged up to values of 3.932 Å and relaxes to bulk values for a film thickness of 170 nm. From capacitance measurements in the temperature range from 293 to 4.2 K we determined the dielectric permittivity for different film thicknesses. An external electric bias field was varied to compensate for internal fields caused by band alignment due to the difference in work function of both electrodes. We discuss the results as a series connection of the film and interface capacitances involving strain effects.

DF 6.11 Tue 9:30 P5

**Micro- and nano-patterning of lithium niobate** — ●THOMAS GISCHKAT<sup>1</sup>, FRANK SCHREMPPEL<sup>1</sup>, HOLGER HARTUNG<sup>2</sup>, ERNST-BERNHARD KLEY<sup>2</sup>, ANDREAS TÜNNERMANN<sup>2</sup>, and WERNER WESCH<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena — <sup>2</sup>Institut für Angewandte Physik, Friedrich-Schiller-Universität Jena

In order to manipulate light on the nanoscale, the engineering and fabrication of novel photonic nanomaterials and devices (e.g. photonic crystals, micro-resonators and Bragg-gratings) using micro- and nanoscale patterning technologies is of growing interest. We report on the patterning of LiNbO<sub>3</sub> by means of Ion Beam Enhanced Etching (IBEE), which is based upon the fact, that the chemical resistance of the crystal is reduced due to ion irradiation induced defects. Thus the irradiated regions can be removed without affecting the non-irradiated crystal. The principle of the method is introduced and the influences of fundamental parameters like ion fluence, irradiation and etching temperature are discussed. Lateral patterning is performed by creation of a damaged- commonly amorphous - layer starting from the surface. To define the lateral geometry, masks prepared by standard lithographic processes applying photo- or electron-beam-lithography are used providing the opportunity for a selective irradiation with ions. Vertical patterning is obtained, if the damage is established as a buried layer. Actually three dimensional patterning is possible if lateral and vertical patterning is performed together. This is exemplarily shown for micro-discs and 2D-photonic crystals with underlying air gap, respectively.

DF 6.12 Tue 9:30 P5

**Ultra-fast detection of multi-wave mixing on optically induced microstructures** — ●ANNIKA KRUSE, BETTINA SCHOKE, and MIRCO IMLAU — Department of Physics, University of Osnabrück, Germany

The ultra-fast detection of multi-wave mixing on optically induced microstructures was examined with iron-doped lithium niobate (LiNbO<sub>3</sub>:Fe) for test purposes. The aim of this work is to analyse contributions of index and absorption gratings in short-living mixed diffraction gratings with a decay time below 10 ms. A standard holographic two-beam setup allowing for the recording and simultaneous reading of elementary gratings in LiNbO<sub>3</sub>:Fe ( $\lambda_{\text{rec}} = 514 \text{ nm}$ ;  $\theta_{\text{rec}} = 20^\circ$ ,  $\lambda_{\text{read}} = 633 \text{ nm}$ ;  $\theta_{\text{B}} = 25^\circ$ ) was applied and expanded by a fast motorized rotary stage (rotation velocity 720°/s) for sample rotation. This enabled the determination of the rocking curve from recorded diffraction gratings, i.e. the angular dependence of the diffraction efficiency on the angular deviation from the Bragg angle was measured. Appropriate photo diodes and a digital storage oscilloscope for data collection were used in order to match for the high scan speed. As a result, the rocking curves could be detected with excellent resolution in an angular range of  $\pm 0.3^\circ$  within  $< 1 \text{ ms}$ . The results are successfully compared with theoretical expectations of mixed diffraction gratings. The continuative development of this technique for a comprehensive two-beam coupling analysis is discussed. \*Financial supported by the Deutsche Forschungsgemeinschaft (Projects IM37/5-1 and GRK 695).

DF 6.13 Tue 9:30 P5

**A Versatile Surface Modification Method for Mesoporous TiO<sub>2</sub>** — ●DEREJE HAILU TAFFA, KATHIRESAN MURUGAVEL, and LORENZ WALDER — Institut für Chemie, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück

Mesoporous titanium dioxide is a large-area, dielectric material used in many applications such as photovoltaics, electrochromics, catalysis and sensors. Many of these applications require a functional molecule anchored to the inner walls of the porous system. We present a new method for the anchoring of such molecules using a combination of hydrophobic and electrostatic interactions. For this purpose we prepared alkyl phosphonic acids of different chain length (6, 10, and 14 carbons) bearing neutral, positive and negatively charged head groups. They were anchored to the inner walls of randomly sintered, mesoporous titanium dioxide thin films. Quartz crystal microbalance and FT-IR measurements show that a monolayer coverage was achieved. Different charged guest molecules (metal complexes and N-alkyl viologens with variable chain length) were incorporated on top or into the supported membranes. The assemblies were characterized by cyclic voltammetry and FT-IR. The new surface modification technique simplifies the molecular requirements for functional surface modifiers considerably. Using a limited set of organic anchors with orthogonal coordination properties and adjustable hydrophobicity, a broad range of electrochromophores, redox active wiring compounds or sensitizers can be adsorbed onto titania.

DF 6.14 Tue 9:30 P5

**Preparation and characterization of [Fe(CN)<sub>5</sub>NO]<sup>2-</sup> electrostatically attached to TiO<sub>2</sub> surfaces** — VOLKER DIECKMANN<sup>1</sup>, ●SEBASTIAN EICKE<sup>1</sup>, MIRCO IMLAU<sup>1</sup>, DEREJE HAILU TAFFA<sup>2</sup>, LORENZ WALDER<sup>2</sup>, and THEO WOIKE<sup>3</sup> — <sup>1</sup>Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — <sup>2</sup>Institute of Chemistry, Center of Interface Science (CIS), University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany — <sup>3</sup>I.

Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln, Germany

Sodium nitroprusside (Na<sub>2</sub>[Fe(CN)<sub>5</sub>NO]) undergoes a photoinduced NO ligand linkage isomerism in bulk crystal and in solution. In the latter case the complex can release NO and CN<sup>-</sup> after photoexcitation with UV or blue-green light. So far nothing is known on the behavior of nitroprusside in thin films. We have introduced a new technique for holding highly charged complexes in a film, and applied it to [Fe(CN)<sub>5</sub>NO]<sup>2-</sup> ions. They are electrostatically attached to a 14-phosphonotetradecane-1-pyridinium, which acts as spacer to the inner walls of a mesoporous TiO<sub>2</sub>-film. A characterization of the system is performed by infrared absorption spectroscopy as well as by electrochemical studies. We are discussing spectral changes during and after light illumination on the background of the photoinduced linkage isomerism, as well as NO and CN<sup>-</sup> release.

DF 6.15 Tue 9:30 P5

**BaTiO<sub>3</sub> nanotubes grown by a sol-gel template method** — ●RICHARD BOUCHER, PETER RENZ, and KI YOON — Institut für Werkstoffwissenschaft, Helmholtzstr. 7, 01062 Dresden

The growth of nanostructures has been thrust into the limelight in recent years due to the great potential that these structures show. Several production strategies exist such as chemical vapour deposition, microlithography and sol-gel. Several advantages exist for the sol-gel route, but here we are concentrating on the possibility that we can produce nanotubes. This growth occurs because during the production process the material is deposited on the template wall and growth occurs from outside inwards. Our interests led us to the investigation of BaTiO<sub>3</sub> in track etched polycarbonate templates. In this work we have used the chemical route of Limmer as the basis. An example of some nanotubes is shown. In our contribution we will discuss the production route, its optimisation, and the use of other templates and/or materials.

DF 6.16 Tue 9:30 P5

**Laser Light Scattering by 3D Phase Lattices** — ●BJÖRN BRÜSER and ULLRICH PIETSCH — Universität Siegen, Siegen, Deutschland

We have investigated recently developed three-dimensional phase lattices with lattice constants in the  $\mu\text{m}$  - regime by means of laser-light diffraction. The samples have been manufactured by multiple beam interference into light-sensitive polymers resulting in a three-dimensional sinusoidally modulated refractive index distribution which differs by no more than  $\Delta n = 0.001$  between maximum and minimum. For reasons of stability these holograms are sandwiched in between two glass-plates. Because of their 3D periodicity and the fact that the lattice parameters are in the micron range the structures can also be described as photonic crystals. The realized crystallographic structure is of hexagonal or rhombohedral (trigonal) symmetry. Due to crystalline symmetry the sample exposure with a coherent white beam of visible light will result in Laue spots of different colour at different incident angles. The degree of colour separation depends on the diffraction order and on the number of periodically stacked hexagonal planes within the sample, in our case ranging from 10 to 30. Experimentally, we have measured the intensity distribution of single Laue-spots in transmission geometry for different incident angles by rotating the sample. Our experimental setup, including a high resolution diffractometer, enables us to obtain extremely precise angular measurements. The diffraction curves have been recorded and compared to a theoretical model based on an x-ray kinematical scattering approach. The validity of this model arises from the fact that there is only little change in the refractive index variation.

## DF 7: Advanced Dielectrics

Time: Tuesday 14:00–16:20

Location: WIL A317

### Invited Talk

DF 7.1 Tue 14:00 WIL A317

**Origins of large piezoelectric response and lead-free alternatives to PZT** — ●DRAGAN DAMJANOVIC — Ceramics Laboratory, Swiss Federal Institute of Technology - EPFL

One of the hottest topics in the field of piezoelectricity is replacement of ubiquitous Pb(Zr,Ti)O<sub>3</sub> ceramics (or PZT) with lead-free materials. The most widely adopted approach in this search for new materials is to look for systems exhibiting the same salient features as good lead-

based piezoelectrics: a morphotropic phase boundary (MPB), a tendency for a large polarization rotation, and a monoclinic phase. The term \*polarization rotation\* has been employed only recently and has now become a synonym, together with monoclinic phases, for large piezoelectric properties. It is suggested here that \*polarization rotation\* is an old concept proposed over thirty years ago to explain enhanced properties of PZT in the MPB region. It is shown, using an example of lead-free material, that in addition to polarization rotation

polarization extension can also lead to large electro-mechanical properties. Substantial theoretical and experimental evidence exist to show that the highest piezoelectric response does not appear in monoclinic phases but in the phase transition regions where polarization either changes direction or appears from the non-polar state. It is proposed that concept of structural instability and associated free energy instability is the most general approach that underlies theoretical results and consistently interprets experimental observations on enhancement of piezoelectric properties. Finally, perspectives of finding lead-free alternatives to PZT among presently investigated systems are discussed.

### 5 min. break

DF 7.2 Tue 14:40 WIL A317

**Electronic transport across single metallic nanowires fabricated through ferroelectric lithography** — ●ALEXANDER HAUSSMANN and LUKAS M. ENG — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

The presence of different surface charges and thus different surface reactivities offers the possibility of exploiting domain-structured ferroelectrics as templates for the assembling of various functional nanostructures. This technique therefore is claimed ferroelectric lithography [1], bearing the power for the controlled bottom-up assembly and integration over large sample areas.

Here, we report on both the assembly and characterisation of noble-metal nanowires that were deposited photochemically at 180° domain walls on 5 mol% Mg-doped congruent LiNbO<sub>3</sub> single crystal templates. After connecting these wires to macroscopic contact leads, ohmic conduction properties were revealed in such wires by recording I-V-characteristics in conjunction to Kelvin probe force microscopy (KPFM) [2]. Furthermore, investigations at high spatial resolution were performed in order to quantify a possible spatial separation between the domain wall and the photochemically reactive zone.

[1] S.V. Kalinin, et al., Nano Letters **2**, 589 (2002)

[2] U. Zerweck, et al., Phys. Rev. B **71**, 125424 (2005)

DF 7.3 Tue 15:00 WIL A317

**Low voltage electron emission from [Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>]<sub>0.72</sub>[PbTiO<sub>3</sub>]<sub>0.28</sub> single crystals induced by ferroelectric polarization switching** — ●OLIVER MIETH<sup>1</sup>, VINAY S. VIDYARTHI<sup>2</sup>, GERALD GERLACH<sup>2</sup>, KATHRIN DÖRR<sup>3</sup>, and LUKAS M. ENG<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Technische Universität Dresden, Germany — <sup>2</sup>Institute for Solid State Electronics, Technische Universität Dresden, Germany — <sup>3</sup>Institute for Metallic Materials, IFW Dresden, D-01069 Dresden, Germany

Here we report on electron emission from [Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>]<sub>0.72</sub>[PbTiO<sub>3</sub>]<sub>0.28</sub> (PMN-PT) thin ferroelectric single crystals at ultra-low voltages down to 20 V per 400 μm thickness, and for up to 10<sup>9</sup> switching cycles. PMN-PT samples were prepared with split gold top electrodes exhibiting a 25 μm wide gap region. Applying a sinusoidal voltage between the two top electrodes and the bottom electrode initiated electron emission from the gap region. The emitted electrons were collected under UHV conditions using two single electron counters arranged under an angle of 90°. Two emission regimes have been identified, which are clearly separated by the onset of complete ferroelectric polarization switching. This is also confirmed by recording nanoscale ferroelectric hysteresis loops by means of Piezoresponse Force Microscopy. The emitted electrons are found to have a broad energy distribution with the maximum kinetic energies reaching 110 eV and 50 eV for applied switching voltages of 140 V and 110 V, respectively. Our results confirm that polarization reversal is the governing mechanism behind the electron emission process.

DF 7.4 Tue 15:20 WIL A317

**Ab initio and atomistic simulation of copper doping in the**

**lead-free ferroelectric perovskite potassium sodium niobate** — ●SABINE KÖRBEI and CHRISTIAN ELSÄSSER — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

Recently lead-free ferroelectric ceramics, one of them the perovskite potassium sodium niobate (KNN), have attracted strong scientific interest for being environmentally friendly materials suitable for piezoelectric devices in applications like actuators and sensors. Various doping elements, for instance copper, have been found to improve the ceramic processing conditions and the piezoelectric properties of KNN significantly. Therefore a theoretical understanding of the effects of these impurities is important.

We employed density functional theory in the local density approximation and atomistic simulations with empirical interatomic potentials to determine the preferred lattice site for copper impurities in KNN, and the influence of the impurities on the energy barriers associated with switching the ferroelectric polarization.

DF 7.5 Tue 15:40 WIL A317

**Lead-free ferroelectric solid solutions from first-principles calculations** — ●SILKE HAYN, MELANIE GRÖTING, and KARSTEN ALBE — Materialwissenschaften, TU Darmstadt, Deutschland

Ferroelectric materials provide a link between electricity and mechanical movement. The technologically relevant materials, like PZT, are solid solutions which exhibit a morphotropic phase boundary (MPB). In an attempt to replace PZT by materials that do not contain toxic lead, a wide variety of solid solutions of lead-free perovskites is under investigation. First-principles calculations can be used to assist or even guide this search involving an enormous number of candidate materials.

In this contribution we present DFT calculations on K<sub>x</sub>Na<sub>1-x</sub>NbO<sub>3</sub>, Bi<sub>1/2</sub>Na<sub>1/2</sub>TiO<sub>3</sub> (pure and doped with BaTiO<sub>3</sub>), BaTiO<sub>3</sub> (pure and doped with BaZrO<sub>3</sub>), and PbMg<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub> and compare them with the standard material PZT. For all these materials cation displacements, tilt angles of oxygen octahedra and electronic transfer are evaluated. Further we investigate substitution effects, ordering and local distortion in detail and compare the results to experimental findings.

DF 7.6 Tue 16:00 WIL A317

**Stretchable pressure sensor made of ferroelectret-elastomer-composite and elastic gold electrodes** — ●MARKUS KRAUSE<sup>1</sup>, INGRID M. GRAZ<sup>1,2</sup>, PETR BARTU<sup>1</sup>, SIMONA BAUER-GOGONEA<sup>1</sup>, SIGURD WAGNER<sup>3</sup>, STÉPHANIE P. LACOUR<sup>2</sup>, and SIEGFRIED BAUER<sup>1</sup> — <sup>1</sup>Soft Matter Physics, Johannes Kepler University, Linz, Austria — <sup>2</sup>Nanoscience Centre, Dept. Of Engineering, University of Cambridge, Cambridge, U.K. — <sup>3</sup>Department of Electrical Engineering, Princeton University, Princeton, NJ, USA

Stretchable electronics recently emerged as a new area of macroelectronics, with applications in consumer goods, mobile appliances and artificial skin for full body tactile sensors. Challenges in research are the development of stretchable sensing materials, capable of recording changes in physical parameters such as temperature or pressure. Here we describe a reversibly stretchable pressure sensor material, where charged polypropylene ferroelectret foams as pressure-sensitive part are embedded in a 1mm thick matrix of a surface microstructured silicone elastomer. For electrical readout, 75 nm thick elastic gold electrodes were evaporated on it. The sensor was fabricated and tested as standalone system and combined with an a-Si:H TFT. Modulations in the source-drain-current reflect the periodically applied pressure signal. Pressure in a range from 10 to 1000 kPa was detected, while the sensor was uniaxially stretched up to 40%. The signal remained stable over the described pressure and stretch ranges and is even high enough to switch the TFT from the OFF to the ON-state. Financial support of the work from the FWF is gratefully acknowledged.

## DF 8: Glass I

Time: Tuesday 10:00–12:40

Location: WIL B321

DF 8.1 Tue 10:00 WIL B321

**Upconversion in fluorozirconate based glass ceramics for high efficiency solar cells** — ●BERND AHRENS<sup>1,2</sup>, BASTIAN HENKE<sup>2</sup>, PAUL T. MICLEA<sup>2,3</sup>, and STEFAN SCHWEIZER<sup>2,3</sup> — <sup>1</sup>Department of Physics,

University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — <sup>2</sup>Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale), Germany — <sup>3</sup>Institute of Physics, Martin-Luther-University of Halle-Wittenberg, Heinrich-Damerow-Str. 4,

06120 Halle (Saale), Germany

Solar cells are unable to use the whole solar spectrum. In particular, sub bandgap photons cannot be absorbed. Materials, which convert in an upconversion process two or more sub bandgap photons into photons with an energy higher than the bandgap energy, are of great interest. Low-phonon energy glasses like fluorozirconate (FZ) glasses are desirable hosts for rare-earth ions such as Er, Ho, Nd, Pr, and Tm because they enable upconverted fluorescence that would be quenched in high-phonon energy glasses. FZ glasses additionally doped with trivalent neodymium and chlorine ions and subsequently annealed show enhanced upconverted fluorescence intensities compared to the as-made samples. The samples were annealed at temperatures up to 290°C to initiate the growth of BaCl<sub>2</sub> nanocrystals therein; the Nd<sup>3+</sup> ion is incorporated in the glass as well as in the nanoparticles. The diameters of the nanocrystals are in the range from a few to several tens of nanometers. The development of glass ceramics doped with Er<sup>3+</sup>, whose optical properties make it a better choice for the application as an upconversion layer on silicon solar cells, is in progress.

DF 8.2 Tue 10:20 WIL B321

**Fluorescence efficiency of samarium-doped glasses and glass ceramics** — ●MARCEL DYRBA<sup>1</sup>, BERND AHRENS<sup>2,3</sup>, PAUL T. MICLEA<sup>1,3</sup>, and STEFAN SCHWEIZER<sup>1,3</sup> — <sup>1</sup>Institute of Physics, Martin-Luther-University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale), Germany — <sup>2</sup>Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — <sup>3</sup>Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale), Germany

Optically active glasses and glass ceramics offer a broad range of applications; the functionality can be modified by appropriate doping and thermal processing performed after the glass production. Fluorescence from samarium in glasses has attracted much attention in the past two decades, in particular for studies on spectral-hole burning, excited state absorption, and laser properties. Samarium can enter the glass matrix either in its divalent form and/or as a trivalent ion.

The most efficient fluorescent glasses are characterized by low-phonon energies, a critical parameter leading to reduced non-radiative losses and thus to increased fluorescence efficiencies. However, the phonon frequency is not only dependent on the composition of the matrix the optically-active ion is incorporated into but also by the size of the matrix; in rare-earth doped nanocrystals an increased fluorescence efficiency is found. In this work, we compare the fluorescence efficiency of Sm<sup>2+</sup>/Sm<sup>3+</sup> in different glass systems such as borate glasses, fluorozirconate glasses, or oxyfluoride glasses.

DF 8.3 Tue 10:40 WIL B321

**Improving up-conversion efficiency of rare earth ions by metallic nanoparticles** — ●STEFAN WACKEROW<sup>1</sup>, MARCEL DYRBA<sup>1</sup>, STEFAN SCHWEIZER<sup>1,2</sup>, GERHARD SEIFERT<sup>1</sup>, and HEINRICH GRAENER<sup>1</sup> — <sup>1</sup>Martin Luther university Halle-Wittenberg, 06120 Halle (Saale), Germany — <sup>2</sup>Fraunhofer Center for Silicon Photovoltaics, 06120 Halle (Saale), Germany

A potential way to increase silicon solar cell efficiency is frequency up-conversion of infrared sunlight which can be done by rare earth ions. A novel approach to enhance the up to now rather low up-conversion rates of rare earth ions in glasses is the inclusion of metallic nanoparticles in the glass. The nanoparticles may increase up-conversion efficiencies by the local near-field enhancement and interaction of the plasmon polaritons with rare earth energy levels.

We are therefore studying the co-doping of glasses with rare earth ions and metallic nanoparticles. Generation of silver nanoparticles in glasses is a two-step process. First, silver ions are brought into the glass by field-assisted ion exchange. Second, these glasses are heated in a hydrogen atmosphere, reducing the silver ions to atoms, which then form silver nanoparticles. This nanoparticle formation has been investigated in commercial rare-earth laser glasses, borate glasses and standard soda lime glass. In order to tune the resonance between plasmon polaritons and the rare earth energy levels, we also modified the nanoparticle shapes from spherical to ellipsoidal by irradiating the samples with intense femtosecond laser pulses.

All modified samples were analyzed by fluorescence measurements.

DF 8.4 Tue 11:00 WIL B321

**Correlation analysis of dielectric polarization noise in glass formers** — ●JENS SCHINDELE, ANDREAS REISER, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

The analysis of dielectric polarization noise is a powerful tool to investigate relaxation processes in dielectric or ionic fluids, glass-forming liquids or glasses. To determine the polarization noise, we measure voltage fluctuations between electrodes immersed in the sample. We show time series analyses of voltage fluctuations of typical glass formers in the temperature range between room temperature and the glass transition temperature. Correlations in space and time probed by a three electrode setup. This enables us to follow the random walk of an effective polarization vector in two dimensions.

DF 8.5 Tue 11:20 WIL B321

**Investigation of the microscopic nature of tunnelling systems in glassy glycerol by using nuclear moments as local probes** — ●MASOOMEH BAZRAFESHAN, CELINE RÜDIGER, GUDRUN FICKENSCHER, ANDREAS FLEISCHMANN, and CHRISTIAN ENSS — Kirchhoff-Institut für Physik, Universität Heidelberg, Germany

At low temperatures many properties of glassy materials can be described in the framework of the standard tunnelling model. It assumes the presence of 2-level systems with a broad distribution of energy splittings  $E$ , which arise from particles of mass  $m$  tunnelling between the wells of a double well potential. Up to today, the microscopic nature of these tunnelling systems, i.e. of the tunnelling particles and the tunnelling motion, is not known. We show that nuclear moments on the tunnelling particle can be used as a probe for the microscopic motion of tunnelling systems. We have performed dielectric polarization echo experiments on a series of partially deuterated glycerol samples. The electric quadrupole moments of the deuterium nuclei interacting with local electric field gradients cause a fine splitting of the tunnelling levels, which leads to a quantum beating in small magnetic fields and a pronounced magnetic field dependence of the echo amplitude. The anisotropic interaction of the magnetic dipole moments of the hydrogen nuclei yields a similar effect on a smaller energy scale. By comparing the data to detailed numerical model calculations we were able to extract an effective tunnelling angle and can draw preliminary conclusions about the microscopic properties of the tunnelling entities.

DF 8.6 Tue 11:40 WIL B321

**Mechanisms of atom dynamics on the microseconds scale during the alpha-decay in MD simulated glass forming Ni<sub>0.5</sub>Zr<sub>0.5</sub>** — ●HELMAR TEICHLER — Institut für Materialphysik, Universität Göttingen, Göttingen, Germany

In glass forming melts near TG, the alpha-decay reflects relaxation processes on meso- and macroscopic time scales. Its microscopic explanation is a challenging open question, as it needs to understand emergence of extreme slow dynamics, more than ten orders of magnitude below atomic vibrations, from the atomic motions in the melt. Here we present molecular dynamics simulation results on the microseconds scale for glass forming Ni<sub>0.5</sub>Zr<sub>0.5</sub> at 785 K, aimed at elucidating the microscopic processes of meso-scale dynamics during the alpha-decay well below the critical temperature T<sub>c</sub> of mode coupling theory. From the self intermediate scattering function we find that avalanches of collectively moving atoms, local in space and time, dominate these dynamics. The avalanches are known as higher organized cooperative processes in high-viscous dynamics [H. Teichler, PRE 71, 031505 (2005); JNCS 312, 533 (2002)], and more recently as "democratic particle motion" [G.A. Appignanesi et al. PRL 96, 057801 (2006)]. From our MD data, avalanches turn out as rare events, being created at or near a preceding one with about microsecond delay. Our results are discussed with regard to the dynamical facilitation model of Garrahan and Chandler.

DF 8.7 Tue 12:00 WIL B321

**Length scale effects in amorphous metals investigated by mechanical loss spectroscopy** — ●DENNIS BEDORF, MORITZ SCHWABE, and KONRAD SAMWER — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Glassy behavior is, in a common assumption, affected by inhomogeneities in internal dynamics. Recent computer studies using molecular dynamics have revealed dynamical heterogeneities on an atomic length scale (Teichler et al., Zink, Mayr[1] and Neudecker). During a shear process shear transformation zones with a radius of about 1.5 nm and string like fluctuations with several nm length occur. Both processes are supposed to be surrounded by an Eshelby-Stress-Field to memorize configuration via the elastic energy [2].

Mechanical spectroscopy using double-paddle-oscillator technique enables us to study mechanical loss in thin films. For this study we

choose glassy PdCuSi. The dependence of the loss on temperature and film thickness delivers the activation of certain processes in particular  $\alpha$ - and  $\beta$ - process (wing). Our measurements show a disappearance of the  $\beta$ - process below 50 nm. We discuss this finding in terms of stress fields competing with spatial confinement and surface annihilation.

This work was supported financially by DFG, SFB 602 and Leibniz Programm.

[1] M. Zink, K. Samwer, W. L. Johnson and S. G. Mayr, Phys. Rev. B 73, 172203, (2006).

[2] J. S. Harmon, M. D. Demetriou, W. L. Johnson and K. Samwer, Phys. Rev. Lett. 99, 135502, (2007).

DF 8.8 Tue 12:20 WIL B321

**Influence of surfaces on dynamics in polymer thin films - a molecular dynamics study** — ●CHRISTIAN VREE and STEFAN GEORG MAYR — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The influence of free surfaces on the mobility of model polymer chains is investigated with the help of classical molecular dynamics simulations. Below a critical temperature,  $T^*$ , a strong enhancement of the mobility of chains near the surfaces is observed, as calculated from the center-of-mass displacements of the chains. This effect diminishes with increasing temperature. A similar behavior is observed in fluctuations of the radius of gyration, corresponding to conformation changes and hence to structural relaxations. Here the difference between surface and bulk decreases with increasing temperature as well as with increasing time. The temporal evolution of these fluctuations give rise to characteristic sampling times and, thus, activation energies of relaxations of the system. The activation energy for surface relaxations is found to be lower than for bulk relaxations and additionally less temperature dependent.

This work is financially supported by the DFG - SFB 602 (TP B3).

[1] C. Vree and S.G. Mayr, submitted to New Journal of Physics (2008)

## DF 9: Glass II

Time: Tuesday 14:00–16:00

Location: WIL B321

DF 9.1 Tue 14:00 WIL B321

**Ion conductivity of Lithium-Borate glass layers in the nanometer thickness range** — ●GERD-HENDRIK GREIWE, FRANK BERKEMEIER, and GUIDO SCHMITZ — Institut für Materialphysik der Westf. Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Specific ion conductivities of thin layers of Lithium-Borate-glasses with the compositions  $x \text{Li}_2\text{O} \cdot (1-x) \text{B}_2\text{O}_3$ , with  $x = 0.15, 0.20, 0.25$  and  $0.35$ , are determined by impedance spectroscopy as a function of temperature and layer thickness. The glass layers are prepared by ion-beam-sputtering in the thickness range from 7 nm up to 1000 nm.

Previous measurements of our group demonstrated a significant increase of the specific conductivity with decreasing layer thickness. The increase is about three orders of magnitude and occurs for layers with a thickness under  $\approx 100$  nm. Recent measurements show that this finite size effect only arises for Aluminium Lithium electrodes. In the case of Aluminium electrodes no significant thickness dependence appears. Therefore diffusion of Lithium from the electrodes into the glass-layers must be assumed as reason for the effect. In the talk different models for the concentration profile of Lithium inside the glass-layers are discussed to explain the observed finite size effect.

DF 9.2 Tue 14:20 WIL B321

**Understanding the nature of ion conductivity in inorganic systems** — ●ANDREAS HEUER<sup>1</sup> and HEIKO LAMMERT<sup>1,2</sup> — <sup>1</sup>Institut für Physikalische Chemie, WWU Münster — <sup>2</sup>Center for Theoretical Biological Physics, San Diego

It is well accepted that the ion dynamics in inorganic ion conductors is based on ionic hops between adjacent sites provided by the network. It can be shown that the number of sites is only slightly larger than the number of ions [1]. Thus, it has been speculated that the ion dynamics should be described as a vacancy rather than a particle dynamics. This approach is elucidated in this contribution. First, a quantification of the vacancy dynamics has to be achieved. Whereas this is trivial for lattice models, several complications arise for continuous systems. In this way one can identify, e.g., the relevance of cooperative ion jumps, corresponding to vacancy jumps beyond the nearest neighbor shell. Second, from studying the distribution of waiting times of a specific site as well as the patterns of forward-backward jumps one finds that the vacancy dynamics can be basically described as a single-particle problem (in contrast to the ionic motion). This result justifies the use of single-particle models such as the random-energy model to describe ion dynamics. Third, it is checked that the macroscopic conductivity can be described within a single-particle approach for the vacancies. [1] H. Lammert, M. Kunow, A. Heuer, Phys. Rev. Lett. 90, 215901 (2003).

DF 9.3 Tue 14:40 WIL B321

**How important are facilitation processes for the dynamics in supercooled liquids?** — ●CHRISTIAN REHWALD and ANDREAS HEUER — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149 Münster

We investigate a binary mixture Lennard-Jones liquid by molecular dynamics simulation with respect to finite size effects. Our focus is the  $q$ -dependent relaxation time  $\tau(q)$  and the diffusion constant  $D$  calculated from particle coordinates, inherent structures and metabasins [1]. It turns out that globally defined metabasins are no longer sufficient to predict  $S(q,t)$  for large systems (except for small  $q$ ). In order to avoid this problem, we calculate *local* exchange time distributions, generated by averaged particle displacements [2]. The locally defined distributions show a similar behavior as that of metabasins for long waiting times without depending explicitly on  $N$ . Moreover, as a result of facilitation processes, increasing the system size leads to a reduction of the long tails of the exchange time distribution. This  $N$ -dependence is exactly the one expected from a model glass-former based on a set of coupled elementary unit systems [3], which is e.g. implemented in several facilitated spin models.

[1] A. Heuer, Phys.: Cond. Mat. 20 (2008)

[2] L. O. Hedges *et al.*, J. Chem. Phys. 127 (2007)

[3] M. Vogel *et al.*, J. Chem. Phys. 120 (2004)

DF 9.4 Tue 15:00 WIL B321

**Glass-Transition Scenarios for the Square-Shoulder System** — ●MATTHIAS SPERL — Institut für Materialphysik im Weltraum, DLR, Koeln

It was discovered recently that the competition of two mechanisms of glassy arrest can trigger glass-glass transitions if the two glasses are sufficiently distinct in their localization length. It was found in simulation and experiment that the interplay between hard-sphere repulsion and a short-ranged attraction can exhibit such a scenario. Here the competition between two repulsive length scales is considered. While for both very low and very high shoulders the hard-sphere limit is recovered, for specific widths and heights of the shoulder one can identify higher-order glass-transition singularities that are indicative of glass-glass transitions. In addition, multiple reentry scenarios are found: glass-liquid-glass transitions are possible both for constant density as well as for constant temperature. The results for the square-shoulder glass transition (and its generalizations) are expected to be relevant in micellar, metallic, and granular systems as well as in water.

This work is done in collaboration with E. Zaccarelli, F. Sciortino, P. Kumar, and H. E. Stanley.

DF 9.5 Tue 15:20 WIL B321

**Lower critical dimension of the spherical spin glass** — ●FRANK BEYER and MARTIN WEIGEL — Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

Considering  $O(n)$  vector spin glasses, a major simplification of the free energy landscape occurs in the limit of an infinite number of spin components ( $n \rightarrow \infty$ ), i.e., for the spherical spin glass. This simplification comes about through the fact that in the limit of a large number of spin components the ground state of a finite system occupies only a finite-dimensional subspace in spin space. As a consequence, for each system size there exists a finite, critical number  $n^*$  of spin components

above which the ground-state energy does not change upon further adding spin dimensions, such that the system effectively describes a spherical spin glass. Here, this observation is exploited for investigating the stability of the ordered phase of the spherical spin glass as a function of the spatial dimension of the lattice. Using the concept of the defect energy, we numerically determine the stiffness exponents for lattices of various spatial dimensions  $d = 2, 3, \dots$  and use these results to estimate the lower critical dimension of the model. The results are compared to estimates resulting from field-theoretic calculations.

DF 9.6 Tue 15:40 WIL B321

**Relaxational dynamics of a fragile plastic crystal investigated by dielectric spectroscopy** — •THOMAS BAUER, MELANIE KÖHLER, PETER LUNKENHEIMER, and ALOIS LOIDL — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

In the present contribution, we report dielectric spectra on 60succinonitrile-40glutaronitrile (60S40GN), a binary mixture showing

an orientationally disordered (OD) plastic-crystal phase with unusually high fragility [1].

Based on earlier works [2], the relaxation dynamics of OD materials generally seem to show rather strong characteristics within the strong-fragile classification scheme by Angell. However, the plastic crystalline phase of 60S40GN behaves unconventional in this respect and can be characterized as fragile [1]. This finding may be ascribed to a higher density of minima in the potential energy landscape, caused by substitutional disorder effects. Furthermore, the presented system is a good ionic conductor, showing decoupling between rotational and translational dynamics. In addition, while most other plastic crystalline phases show no or only a very weak secondary process [2], 60S40GN exhibits a well developed  $\beta$  relaxation.

[1] F. Mizuni, J.-P. Belieres, N. Kuwata, A. Pradel, M. Ribes, and C.A. Angell, *J. Non-Cryst. Solids* 352, 5147 (2006).

[2] See, e.g., R. Brand et al., *Phys. Rev. Lett.* 82, 1951 (1999); R. Brand et al., *J. Chem. Phys.* 116, 10386 (2002).

## DF 10: Photonic Dielectrics I

Time: Wednesday 10:00–12:40

Location: WIL A317

### Invited Talk

DF 10.1 Wed 10:00 WIL A317

**Photoswitchable Complexes: Properties and Applications** — •DOMINIK SCHANIEL — I. Physikalisches Institut, Universität zu Köln

Photorefractive and photochromic materials are used in a variety of applications. This contribution reviews the properties and reports recent progress with respect to applications of unconventional photorefractive materials, based on photoswitchable complexes. Emphasis will be laid on compounds, in which ligands such as NO, NO<sub>2</sub>, SO<sub>2</sub>, and (CH<sub>3</sub>)<sub>2</sub>SO can be switched by light [1-3]. In these materials large photorefractive and photochromic responses can be induced on ultrashort timescales. The use of the complexes in various states of matter (liquid, solid, hybrid and nanomaterials) allows for tuning of the photorefractive/photochromic properties and thus paves the way for a targeted design of optical devices.

[1] D. Schaniel et al., *Adv. Mater.* 19, 723 (2007). [2] J. M. Cole, *Z. Kristallogr.* 223, 363 (2008). [3] J. J. Rack, *Z. Kristallogr.* 223, 356 (2008).

### 5 min. break

DF 10.2 Wed 10:40 WIL A317

**Photoswitchable [Ru(bpy)<sub>2</sub>(OSO)]PF<sub>6</sub> molecules for nonlinear opto-fluidics** — •VOLKER DIECKMANN<sup>1</sup>, SEBASTIAN EICKE<sup>1</sup>, MIRCO IMLAU<sup>1</sup>, NICHOLAS V. MOCKUS<sup>2</sup>, THEO WOIKE<sup>2</sup>, and JEFFREY J. RACK<sup>3</sup> — <sup>1</sup>Department of Physics, University of Osnabrück, Barbarastr. 7, D-49069 Osnabrück — <sup>2</sup>I. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln — <sup>3</sup>Department of Chemistry and Biochemistry, Ohio University, Athens, Ohio 45701

The studies on [Ru(bpy)<sub>2</sub>(OSO)]PF<sub>6</sub> (OSO: 2-methylsulfinylbenzoate) characterize the photoswitchability of the molecules concerning the activation energy, the spectral range and the lifetime of the excited states at room temperature. The kinetics of the generation of excited states and their thermal decay were determined by pump-probe technique: The absorption of the solution was probed by 532 nm light during and after pumping with 405 nm light. Two fully reversible thermal decay processes following Arrhenius law ( $E_{A,I} = (1.0 \pm 0.2)$  eV and  $E_{A,II} = (0.7 \pm 0.1)$  eV) have been identified. Additionally, absorption spectroscopic studies reveal a photosensitivity and strong absorption changes in the UV spectral range. The lifetimes of the photo-excited states in [Ru(bpy)<sub>2</sub>(OSO)]PF<sub>6</sub> solutions at room temperature have been determined to  $\tau_I \approx 1.4 \cdot 10^5$  s and  $\tau_{II} \approx 4 \cdot 10^3$  s, respectively. In conclusion, this compound extends the class of photoswitchable molecules to molecules with long lifetimes at room temperature. The application of [Ru(bpy)<sub>2</sub>(OSO)]PF<sub>6</sub> for nonlinear optofluidic systems will be discussed taking into account tuning ability of lifetime and spectral sensitivity. Financial support by the DFG (GRK 695).

DF 10.3 Wed 11:00 WIL A317

**Solid-state dye materials** — •JENNIFER KRAUSE, ANDREA SCHUY, ROBERT LEPSKI, and DOMINIK SCHANIEL — I. Physikalisches Institut, Universität zu Köln, Köln, Germany

Solid-state dye materials are highly requested for applications in tunable lasers or as luminescent materials. We synthesized solid-state dye materials by embedment of organic dyes into anorganic silica matrices and characterized them by absorbance and luminescence spectroscopy. The influence of the matrix parameters like pore size and pH-value as well as the concentration dependence on the luminescence properties has been determined. Furthermore the photostability was compared to that of liquid dyes and embedded in other matrix materials.

DF 10.4 Wed 11:20 WIL A317

**Lithiumniobat-Nanopartikel für optische Anwendungen\*** —

•DANIEL SCHÜTZE, BASTIAN KNABE and KARSTEN BUSE — Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn

Die Kombination von Lithiumniobat-Nanopartikeln mit Trägermaterialien, z. B. Flüssigkeiten, verspricht, Hybridmaterialien mit variablen ferroelektrischen und optischen Eigenschaften zu erzeugen. Wir demonstrieren einen nass-chemischen Ansatz zur Herstellung von Lithiumniobat-Nanopartikeln mit einer angestrebten Größe von 20 nm. Die erzeugten Proben werden mit Hilfe dynamischer Lichtstreuung, Transmissionselektronenmikroskopie und Spektroskopie charakterisiert.

\*Wir danken der DFG und der Deutschen Telekom AG für finanzielle Unterstützung.

DF 10.5 Wed 11:40 WIL A317

**Strahlungsinduzierte Modifikationen des Polungsverhaltens von magnesiumpulvertem Lithiumniobat** — •LENA JENTJENS<sup>1</sup>, KONRAD PEITHMANN<sup>1</sup>, KARL MAIER<sup>1</sup>, HENDRIK STEIGERWALD<sup>2</sup> und TOBIAS JUNGK<sup>2</sup> — <sup>1</sup>Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn — <sup>2</sup>Physikalisches Institut, Universität Bonn

Auf Grund des stark unterdrückten photorefraktiven Effektes ist mit Magnesium dotiertes Lithiumniobat (LiNbO<sub>3</sub> : Mg) für viele Anwendungen interessant. In periodisch gepoltem Lithiumniobat (PPLN) kann über Quasi-Phasen-Anpassung eine effiziente Frequenzverdopplung erreicht werden, welche in LiNbO<sub>3</sub> : Mg selbst bei höchsten Laserintensitäten funktioniert.

Durch die Bestrahlung mit schnellen <sup>3</sup>He-Ionen mit einer Energie von 41 MeV können entscheidende Materialeigenschaften gezielt geändert werden. In der durchstrahlten Region (vor dem Bragg-Peak) werden langzeitstabile Brechungsindexänderungen von bis zu  $6 \times 10^{-3}$  beobachtet. Des Weiteren wird das ferroelektrische Koerzitivfeld  $E_C$  um etwa 10% vermindert und dadurch eine Invertierung der Domänen erleichtert. Durch die Bestrahlung wird zudem die Erzeugung von PPLN mit Periodenlängen im  $\mu$ m-Bereich erleichtert, die für die Frequenzverdopplung von blauem Laserlicht benötigt wird.

DF 10.6 Wed 12:00 WIL A317

**Conductivity through an organic field-effect transistor with ferroelectric gating** — •TIM KUNZE<sup>1</sup>, SYBILLE GEMMING<sup>1</sup>, REGINA LUSCHTINETZ<sup>2</sup>, VOLKER PANKOKE<sup>1</sup>, and MICHAEL SCHREIBER<sup>3</sup> — <sup>1</sup>Forschungszentrum Dresden-Rossendorf, P.O. Box 51 01 19, D-01314

Dresden, Germany — <sup>2</sup>Physical Chemistry and Electrochemistry, TU Dresden, D-01062 Dresden, Germany — <sup>3</sup>Institute of Physics, TU Chemnitz, D-09107 Chemnitz, Germany

The electronic transport of electrons and holes through stacks of functionalized quaterthiophene molecules as part of a novel organic ferroic field-effect transistor is investigated. The novel application of a ferroelectric instead of a dielectric substrate provides a bit-wise switching of the ferroelectric domains and enables the opportunity of employing the polarization field of these domains as a gate field in an organic semiconducting device. An already established phenomenological model called multilayer organic light-emitting diodes (MOLED) [1] is extended to transverse fields and numerical results are discussed. Model-specific parameters are determined with the help of experimental and theoretical methods.

[1] Houili et al., *Comp. Phys. Comm.* 156, 103-122 (2003)

DF 10.7 Wed 12:20 WIL A317

**E-Feld-generierte Abdrücke von Submikrometer-Strukturen auf Glas-Silber-Nanokompositen** — ●MORITZ BELEITES, STEFAN WACKEROW, HEINRICH GRAENER und GERHARD SEIFERT — Fachbe-

reich Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle

Metallische Nanopartikel in Glas können durch Anlegen eines elektrischen Feldes bei erhöhter Temperatur zu Ionen aufgelöst werden (EFAD = electric field-assisted dissolution), wobei entsprechende nanoskopische Hohlräume im Glas zurück bleiben. Verwendet man als Anode eine 2-dimensional strukturierte Elektrode, so kann bei diesem Prozess die Struktur als Höhenprofil auf das Glas-Silber-Nanokompositmaterial übertragen werden. Beispielsweise entstand bei Verwendung eines photonischen Kristalls aus Si (quadratische Löcher senkrecht zur Oberfläche, Strukturperiode  $2\mu\text{m}$ ) ein fast perfekter Abdruck der Struktur mit einer typischen Höhenmodulation von  $\approx 10\text{nm}$ .

Um zu klären, ob dieses Höhenprofil bevorzugt durch das Kollabieren der Nanoporen oder den Ionentransport durch das während des Prozesses an der Probe anliegenden elektrischen Feldes entsteht, wurden die Oberflächen verschiedener Proben nach EFAD mit Hilfe von Rasterkraft-Mikroskopie untersucht. Der Vergleich mit Glaszusammensetzung und den entsprechenden Prozessparametern deutet darauf hin, dass die Ionenwanderung dominiert.

## DF 11: Photonic Dielectrics II

Time: Wednesday 14:30–17:10

Location: WIL A317

### Invited Talk

DF 11.1 Wed 14:30 WIL A317

**Real-time probing of structural dynamics in perovskite materials** — ●THOMAS ELSAESSER — Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, D-12489 Berlin, Germany

Femtosecond x-ray diffraction probes structural dynamics of solids in real-time and gives insight into reversible geometry changes on atomic length and time scales. After a brief introduction into this field, recent results on the lattice dynamics of ferroelectric  $\text{SrRuO}_3/\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  superlattice structures and their interplay with the electric polarization of the material are presented [1]. Ultrafast optical generation of mechanical stress allows for switching-off the polarization on a time scale of a few picoseconds. As a second example, magnetostriction in a ferromagnetic  $\text{SrRuO}_3/\text{SrTiO}_3$  superlattice structure is analyzed in real time [2].

[1] C. von Korff Schmising et al., *Phys. Rev. Lett.* 98, 257601 (2007)

[2] C. von Korff Schmising et al., *Phys. Rev. B* 78, 060404(R) (2008)

### 5 min. break

DF 11.2 Wed 15:10 WIL A317

**Ultrafast shape transformation dynamics of silver nanoparticles studied by femtosecond pulse-pair irradiation** — ●AKIN ÜNAL, ANDREI STALMASHONAK, GERHARD SEIFERT, and HEINRICH GRAENER — Institut für Physik, Fachgruppe Optik, Martin-Luther-Universität, Hoher Weg 8, 06120 Halle, Germany

Spherical silver nanoparticles embedded in glass were irradiated by pairs of time-delayed laser pulses with equal intensities resulting in delay-dependent nanoparticle shape transformations. The corresponding permanent changes of the surface plasmon extinction bands are analyzed as a function of time delay and relative polarization of the pulse pairs. We find that the strongest nanoparticle shape changes, i.e. the highest aspect ratios, are achieved when the delay between pulse pairs is less than 3 ps. After 10 ps the aspect ratio is strongly reduced in the case of pulse pairs having identical polarization and vanishes using pulse pairs with orthogonal polarization. Estimations of the time dependence of "pulse-enhanced" (directed) and thermal (isotropic) electron emissions obtained from an extended two-temperature model indicate a decay of the relative contribution of directed electron emission on the same time scale of a few picoseconds. Our results strongly suggest that the electron and following ion emission from the nanoparticles are finished within less than 20 ps, and the directional memory is favorably defined by directed emission of hot electrons interacting with the laser field.

DF 11.3 Wed 15:30 WIL A317

**Femtosecond white-light pump-probe investigation of laser-induced shape transformation of silver nanoparticles in glass** — ●ARMIN WARTH, GERHARD SEIFERT, JENS LANGE, and HEINRICH GRAENER — Fachbereich Physik, Martin-Luther-Universität Halle-

Wittenberg, 06120 Halle

Soda lime-glasses containing spheroidal silver nanoparticles are used as the base material for production of high-quality polarisers, dichroic optical microstructures or long-time optical data storage. Permanent shape transformation of the nanoparticles can be induced by irradiation with intense femtosecond laser pulses. The most efficient transformation to spheroids with large aspect ratio is achieved in 'multi-shot mode', where several hundred laser pulses in the range of 0.2 - 0.5  $\text{TW}/\text{cm}^2$  on average hit one spot on the sample.

To study the ultra short dynamics of such irreversible, shot-by-shot increasing changes, we introduce a highly efficient femtosecond pump - supercontinuum probe setup, which allows us to monitor the changes of optical density with single shot precision. Thus we obtain the complete temporal evolution of spectral changes for each of the several hundred laser shots separately. I.e., after only one measurement cycle we end up with a data set that needs typically 3GB space for data storage. Examples for the results of these experiments are presented and discussed.

DF 11.4 Wed 15:50 WIL A317

**Photorefraktive Gitter in Lithiumniobat-Kristallen erzeugt mit Femtosekunden-Laserpulsen\*** — ●DOMINIK MAXEIN, JOHANNA BÜCKERS, DANIEL HAERTLE und KARSTEN BUSE — Physikalisches Institut, Wegelerstr. 8, D-53115 Bonn, Deutschland

Der photorefraktive Effekt in Lithiumniobat-Kristallen ( $\text{LiNbO}_3$ ) bietet einerseits die Möglichkeit, Brechungsindexstrukturen und diffraktive optische Elemente in  $\text{LiNbO}_3$  einzuschreiben. Andererseits kommt es durch unerwünschte Brechungsindexänderungen zu „lichtinduzierter Streuung“ und zum „optischen Schaden“, was Anwendungen der Kristalle behindert.

Insbesondere nichtlineare Anwendungen gehen meist mit hohen Intensitäten einher. Darum ist es interessant, den photorefraktiven Effekt mit den hohen Intensitäten und kurzen Anregungszeiten von Femtosekunden-Pulsen zu untersuchen. Dazu werden bei 532 nm mit fs-Laserpulsen und mit cw-Laserlicht Brechungsindex-Gitter in eisen-dotiertes  $\text{LiNbO}_3$  geschrieben und die Beobachtungen verglichen: Die Sättigungswerte der Brechungsindexänderungen verringern sich mit steigender Pulsenergie, was durch die Ein- und Zwei-Zentren-Modelle nicht vorhergesagt wird. Eine Verringerung des  $\text{Fe}^{2+}$ -Gehalts der Kristalle durch Oxidation erhöht die Schreibzeiten mit cw-Licht deutlich, während sie für fs-Pulse weitgehend unverändert bleiben. Mögliche Anregungs- und Ladungstransportmechanismen werden diskutiert, um die Ergebnisse zu erklären.

\*Wir danken der DFG und der Deutschen Telekom AG für finanzielle Unterstützung.

DF 11.5 Wed 16:10 WIL A317

**Photo-induced light scattering of femtosecond laser pulses in iron-doped lithium niobate crystals\*** — ●JOHANNA BÜCKERS,

DOMINIK MAXEIN, DANIEL HAERTLE, and KARSTEN BUSE — Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany

Lithium niobate is an advantageous material for photonics, e.g., holographic spectral filtering, optical image processing, and holographic diffraction can be realized. However, since lithium niobate crystals are photorefractive, illumination of the crystals is accompanied with undesirable effects like the “optical damage” and “photo-induced light scattering”. Photo-induced light scattering leads to a loss of the transmitted light because of the self-amplification of weak scattered coherent light waves. Consequently, it causes a distortion of the beam shape of the incoming light wave and, thus, hinders photonic applications.

Our investigations show that for femtosecond laser pulses the light-induced scattering is reduced in  $\text{LiNbO}_3:\text{Fe}$  in comparison to illumination with cw laser light at 532 nm. Moreover, it is completely absent for femtosecond pulses in samples with sufficiently small  $\text{Fe}^{2+}$  content, in contrast to the scattering of cw light. Further differences are reflected in a slower buildup time, a narrower angular distribution of the scattered light, and a weaker Bragg selectivity for pulsed illumination. These characteristics can be attributed to the shorter coherence length of femtosecond pulses.

\*Financial support from the Deutsche Forschungsgemeinschaft (FOR 557) and the Deutsche Telekom AG is gratefully acknowledged.

DF 11.6 Wed 16:30 WIL A317

**Ab-initio determination of the pathways of laser-induced non-thermal melting of InSb** — ●JESSICA WALKENHORST, EEUWE S. ZIJLSTRA, and MARTIN E. GARCIA — Theoretische Physik, Fachbereich Naturwissenschaften, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

We performe ab-initio calculations and dynamical simulations to explain the pathways of ultrafast non-thermal melting in InSb during the first 100's of femtoseconds after intense femtosecond laser excitation. We compute the potential energy surface of femtosecond-laser-excited InSb along the directions in which the crystal becomes soft. Using dy-

namical simulations the time dependence of the atomic coordinates is obtained. We find that at high excitation densities the anharmonicity of the potential energy surface becomes significant after  $\approx 100$  fs. On the basis of our results we explain recent timeresolved x-ray diffraction experiments as reported by Lindenberg et al. [A. M. Lindenberg et al., Science 308, 392 (2005)]. Furthermore we compute the atomic density evolution in time after the laser excitation.

DF 11.7 Wed 16:50 WIL A317

**Determination of the light-induced absorption by transient grating spectroscopy** — ●HAUKE BRÜNING, BETTINA SCHOKE, and MIRCO IMLAU — Department of Physics, University of Osnabrück, Germany

Transient absorption spectroscopy is a well-known pump-probe technique for the study of optically-induced photochromic properties showing decay times in the ms and  $\mu\text{s}$  range. The spectral and temporal behavior of the light-induced absorption is determined from the transmission of white light or probe laser beams. Therefore, single intense laser pulses with a spatially homogeneous intensity distribution have to be applied for the pump process. In contrast, transient grating spectroscopy accounts for light diffraction from an optically-induced absorption grating recorded with spatially modulated pump light using a two-beam interferometer. For grating analysis, the probe-light diffraction efficiency is determined as a function of time and wavelength. Here we demonstrate the possibility to determine the light-induced absorption from transient grating spectroscopy in lithium niobate crystals as an example. Experimental results are presented for the particular case of the presence of mixed photochromic and photorefractive gratings, i.e. light-induced refractive-index changes contribute to the light diffraction as well. Theoretical considerations based on wave-mixing theory allowing for a comprehensive grating analysis are presented. Advantages of the procedure are discussed by comparison with results determined from transient absorption spectroscopy. \*Financial support by the DFG (Projects IM37/5-1 and GRK 695).

## DF 12: Poster II

Time: Wednesday 9:30–12:30

Location: P5

DF 12.1 Wed 9:30 P5

**Cr doping of epitaxial  $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  films** — ●LUDWIG FEIGL<sup>1</sup>, ECKHARD PIPPEL<sup>1</sup>, IONELA VREJOIU<sup>1</sup>, RÜDIGER-A. EICHEL<sup>2</sup>, EMRE ERDEM<sup>2</sup>, ROLAND MATTHEIS<sup>3</sup>, MARIN ALEXE<sup>1</sup>, and DIETRICH HESSE<sup>1</sup> — <sup>1</sup>Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — <sup>2</sup>Institut für Physikalische Chemie I, Universität Freiburg, D-79104 Freiburg, Germany — <sup>3</sup>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  $\text{Pb}_{1.1}\text{Zr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  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  $\text{SrRuO}_3$  electrode grown on a vicinal (100)  $\text{SrTiO}_3$  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<sup>1</sup>, RALF STEINHAUSEN<sup>1</sup>, HORST BEIGE<sup>1</sup>, REINHARD KRÜGER<sup>2</sup>, TOBIAS MÜLLER<sup>2</sup>, UTA HELBIG<sup>2</sup>, DIETER SPORN<sup>2</sup>, CARSTEN SCHUH<sup>3</sup>, STEFAN DENNELER<sup>3</sup>, and HUGO SCHLICH<sup>4</sup> — <sup>1</sup>Martin-Luther-University Halle, Physics Department, PFM, 06099 Halle — <sup>2</sup>Fraunhofer ISC, Würzburg — <sup>3</sup>Siemens AG, CT MM 2, Munich — <sup>4</sup>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  $\approx 1\mu\text{m}$ ). The fibres were embedded in a polymer for characterisation. The resulting 1–3-composites were poled with a DC voltage for 1½ hours. By applying a bipolar sinusoidal voltage with high amplitude (7kV/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  $\text{BiCrO}_3$  thin films** — ●DENNY KÖHLER<sup>1</sup>, ULRICH ZERWECK-TROGISCH<sup>1</sup>, CHRISTIAN LOPPACHER<sup>3</sup>, STEPHAN GEPRÄGS<sup>2</sup>, SEBASTIAN T. B. GÖNNENWEIN<sup>2</sup>, RUDOLF GROSS<sup>2</sup>, and LUKAS M. ENG<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden — <sup>2</sup>Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, München — <sup>3</sup>Laboratoire de Matériaux et Microélectronique de Provence, Universités Paul Cézanne, Marseille

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  $\text{BiCrO}_3$  thin films on the nm length scale. In addition, we investigated the ferroelectric properties of  $\text{BiCrO}_3$  thin films by Piezoresponse Force Microscopy (PFM) and compared them to macroscopic hysteresis mea-



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<sub>3</sub>. We compare the local PFM measurements with the global properties of the BiCrO<sub>3</sub> 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 fourth 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<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>)<sub>2</sub>(CuCl<sub>2</sub>)<sub>2</sub>·2H<sub>2</sub>O 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<sub>1-x</sub>Cr<sub>x</sub>P<sub>2</sub>S<sub>6</sub> single crystals** — ●VLADIMIR SHVARTSMAN<sup>1</sup>, PAVEL BORISOV<sup>1</sup>, YULIAN VYSOCHANSKII<sup>2</sup>, and WOLFGANG KLEEMANN<sup>1</sup> — <sup>1</sup>Angewandte Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — <sup>2</sup>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<sup>I</sup>B<sup>III</sup>P<sub>2</sub>S<sub>6</sub> (A<sup>I</sup> and B<sup>III</sup> are mono- and trivalent metal ions). In particular, CuInP<sub>2</sub>S<sub>6</sub> is in a ferroelectric state below 310 K, while CuCrP<sub>2</sub>S<sub>6</sub> 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<sub>1-x</sub>Cr<sub>x</sub>P<sub>2</sub>S<sub>6</sub> (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<sub>2</sub>P<sub>2</sub>S<sub>6</sub>** — ●KONSTANTIN RUSHCHANSKII<sup>1</sup> and YULIAN VYSOCHANSKII<sup>2</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advance Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — <sup>2</sup>Institute for Solid State Physics and Chemistry, Uzhgorod National University, 54 Voloshyn St., 88000 Uzhgorod, Ukraine

Monoclinic Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub> is a proper uniaxial 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 coexistence 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<sub>1-x</sub>Ba<sub>x</sub>TiO<sub>3</sub> multiferroics** — ●KONSTANTIN RUSHCHANSKII<sup>1</sup>, MARJANA LEŽAIĆ<sup>1</sup>, and NICOLA SPALDIN<sup>2</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advance Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — <sup>2</sup>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<sub>3</sub> 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 EuTiO<sub>3</sub> and BaTiO<sub>3</sub> perovskite oxides. While pure EuTiO<sub>3</sub> is a quantum paraelectric which also exhibits antiferromagnetic properties, mixed Eu<sub>1-x</sub>Ba<sub>x</sub>TiO<sub>3</sub> 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<sub>3</sub> and ordered Eu<sub>1-x</sub>Ba<sub>x</sub>TiO<sub>3</sub> compounds for x > 0.2. We have found a significant Eu off-centering both in the mixed compounds and in pure EuTiO<sub>3</sub>. The influence of hydrostatic pressure on polarization in Eu<sub>1-x</sub>Ba<sub>x</sub>TiO<sub>3</sub> 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<sub>3</sub>)<sub>4</sub>]<sub>2</sub>CuCl<sub>4</sub> crystal** — ●IVAN KARPA — Ivan Franko Lviv National University, Department of Electronics, Non-linear Optics Chair

Investigations of sample size of [N(CH<sub>3</sub>)<sub>4</sub>]<sub>2</sub>CuCl<sub>4</sub> 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<sup>1,2</sup>, T. LEISEGANG<sup>1</sup>, H. STÖCKER<sup>1</sup>, T. WEISSBACH<sup>1</sup>, S. GEMMING<sup>2</sup>, and D.C. MEYER<sup>1</sup> — <sup>1</sup>Institute of Structural Physics, TU-Dresden, 01062 Dresden, Germany — <sup>2</sup>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) *P*<sub>42</sub>/*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*<sub>ij</sub>. 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<sup>3</sup> wafers in (001), (110) and (111) orientation and  $\Psi$ -scans were measured for the reflections 001, 220, 110 and 111. Ti occupies Wyckoff site 2a, its tensor symmetry must follow the local symmetry *m.mm* leaving 3 complex elements *f*<sub>11</sub>, *f*<sub>12</sub>, *f*<sub>33</sub>. The measured data show clear evidence of AAS and the 001 FRED and 111 intensities could be fitted to obtain *f*'<sub>12</sub> and *f*'<sub>12</sub>. Since *f*<sub>13</sub> and *f*<sub>23</sub> 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<sub>0.6</sub>Sr<sub>0.4</sub>)TiO<sub>3</sub> on conducting PdCoO<sub>2</sub>** — ●STEFAN HIRSCH<sup>1</sup>, PHILIPP KOMISSINSKIY<sup>1</sup>, XIANGHUI ZHOU<sup>2</sup>,

CLAUDIA FASEL<sup>3</sup>, and LAMBERT ALFF<sup>1</sup> — <sup>1</sup>Dünne Schichten, Materialwissenschaft TU-Darmstadt, Darmstadt, Deutschland — <sup>2</sup>Forschungszentrum Karlsruhe, Karlsruhe, Deutschland — <sup>3</sup>Disperse Feststoffe, Materialwissenschaft TU-Darmstadt, Deutschland

(Ba<sub>0.6</sub>Sr<sub>0.4</sub>)TiO<sub>3</sub> is investigated intensively due to its promising properties as a tuneable dielectric material with applications e.g. in tuneable filters, multi band antennas and high frequency components. High quality (Ba<sub>0.6</sub>Sr<sub>0.4</sub>)TiO<sub>3</sub> (abbreviated: BST60) thin films were grown on SrTiO<sub>3</sub> and NdGaO<sub>3</sub> 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<sub>2</sub> as a conductive layer and BST60 on top as a dielectric one is grown by pulsed laser deposition. The powder for PdCoO<sub>2</sub> was also produced by a solid state procedure from PdCl<sub>2</sub> 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<sup>1</sup> and WOJCIECH WANARSKI<sup>2</sup> — <sup>1</sup>Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland — <sup>2</sup>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<sub>2</sub>)<sub>2</sub>). 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 monocystal.

DF 12.12 Wed 9:30 P5

**Radioluminescence Investigations on Alumosilicates for Age Determination** — •SUSANNE S. PFEIFER and MATTHIAS R. KRIBETSCHKEK — 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<sup>1</sup>, CLAUS-HENNING SOLTERBECK<sup>1</sup>, VLADIMIR ZAPOROJTCHEK<sup>2</sup>, FRANZ FAUPEL<sup>2</sup>, and MOHAMMED ES-SOUNI<sup>1</sup> — <sup>1</sup>Institute for Materials and Surface Technology, University of Applied Sciences Kiel — <sup>2</sup>Chair for Multicomponent Materials, Christian-Albrechts-Universität zu Kiel

Investigations of film formation of Pb(Zr<sub>0.52</sub>Ti<sub>0.48</sub>)O<sub>3</sub> (PZT) on Pt (111) shows that an interfacial intermetallic layer, Pt<sub>x</sub>Pb, 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<sup>1</sup>, SABINE KERN<sup>1</sup>, CHRISTOPH PIENTSCHKE<sup>1</sup>, HORST BEIGE<sup>1</sup>, FRANK CLEMENS<sup>2</sup> and JULIANE HEIBER<sup>2</sup> — <sup>1</sup>Martin-Luther-Universität Halle-Wittenberg, Halle, Deutschland — <sup>2</sup>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 Compositeigenschaften.

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 Dehnungsfeldstärke-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<sup>1</sup>, KLAUS WANDEL<sup>1</sup> and DIRK NÜSSLER<sup>2</sup> — <sup>1</sup>Institut für Theoretische u. Physikalische Chemie, Wegelerstr. 12, 53115 Bonn — <sup>2</sup>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 Mehrfachreflexionen, 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.

## DF 13: Thin Films and Nanostructures I

Time: Wednesday 14:40–17:00

Location: WIL B321

DF 13.1 Wed 14:40 WIL B321

**Effects of microstructure on electric properties in BiFeO<sub>3</sub> – RMnO<sub>3</sub> thin films** — •CLAUS-HENNING SOLTERBECK, ABDELILAH LAHMAR, SALAH HABOUTI, and MOHAMMED ES-SOUNI — Institute for Materials and Surface Technology, University of Applied Sciences Kiel, Germany

The interplay between structural and electric properties of BiFeO<sub>3</sub> (BFO) is not completely understood. For this comparative study, BFO thin films were grown by a sol-gel spin-coating method with incorporation of rare earth manganites (RMnO<sub>3</sub>). The structure-property correlation is traced by several microscopic methods, but mainly with conductive-tip atomic force microscopy. For our non-epitaxial films, we investigate the effects of co-doping with RE-manganites on the local electric behaviour of the thin films, and we discuss it with respect to pure BFO.

DF 13.2 Wed 15:00 WIL B321

**The influence of charged traps on leakage current through thin dielectric films** — •GRZEGORZ KOZŁOWSKI, JAROSŁAW DABROWSKI, PIOTR DUDEK, GUNTHER LIPPERT, GRZEGORZ LUPINA, and HANS-JOACHIM MÜSSIG — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

We consider a problem of tunneling effect through a dielectric film with a certain distribution of charged traps inside. The transmission coefficient is calculated directly from the one dimensional stationary Schrödinger equation. Correction compensating the charge inhomogeneity in the film (charged defect) as well as the effect of image potential on a tunnelling carrier was included in the calculation. Since trap position in film determines the life time of carriers on a resonant state in defect, for traps in the bulk of the material a typical resonant tunneling takes place. On the other hand, as trap is moved towards the electrode (anode), the influence of resonant state on leakage becomes weaker. For defects in vicinity of anode, the effect of lowering the potential barrier due to the presence of charged defect is dominating and we observe the effective shortening of tunneling path. In this case a material can be treated as ideal film with a certain interface roughness. In order to reveal a typical behavior of all investigated mechanisms, additionally a detailed analysis of current in different regimes of applied voltage was performed. The results are compared with experimental data.

DF 13.3 Wed 15:20 WIL B321

**Humidity effects on electrical properties and thickness of P(VDF-TrFE) films.** — •GENNADY VIZDRIK, BJÖRN MARTIN, and HERBERT KLIEM — Saarland University, Germany

By the Langmuir-Blodgett technique films of P(VDF-TrFE) with 30 and 50 transfers are deposited onto a glass substrate. The films with ellipsometrically determined thicknesses of 56 nm and 75 nm absorb water. Between 10% and 100% relative humidity (r.h.) of the atmosphere the thickness change is less than 2% in accordance with [1]. Using DC measurements at capacitor structures with aluminum electrodes of the area of 1x1 mm square it turns out that water desorption from the saturated state to the dry state takes place in less than 1000 sec. The electrical properties are changed drastically by the absorbed water. In dry samples we find true ferroelectric hysteresis loops, whereas in samples exposed to 100% r.h. a space charge polarization prevails. The remanent polarization is increased by a frequency dependent factor of up to 10. Measurements of the complex permittivity are carried out in the range 0.01 Hz < f < 1 MHz. The imaginary part and the real part increase towards low frequencies. This increase is the more pronounced the higher the r.h. of the atmosphere is. A quantitative comparison of the measured DC conductivity with the permittivity confirms that a space charge polarization effect is responsible for the increase of the permittivity at low frequencies.

[1] P. A. Jacobson et al., App. Phys. Lett., 84, 88, 2004

DF 13.4 Wed 15:40 WIL B321

**Electrical characterization of ferroelectric tunnel junctions with ferromagnetic electrodes** — •MARIO DISCH<sup>1</sup>, ADRIAN PETRARU<sup>1</sup>, MICHAEL HAMBE<sup>2</sup>, MARKUS HEIDELMANN<sup>1</sup>, MARTINA LUYBERG<sup>1</sup>, FALK AMTHOR<sup>1</sup>, RAINER WASER<sup>1</sup>, NAGARAJAN VALANOOR<sup>2</sup>, and HERMANN KOHLSTEDT<sup>1</sup> — <sup>1</sup>Institut für Festkörper-

forschung, Forschungszentrum Jülich GmbH, Jülich, Germany — <sup>2</sup>School of Materials Science and Engineering, University of New South Wales, Sydney, Australia

Heterostructures of SrTiO<sub>3</sub>(substrate)/SrRuO<sub>3</sub>/BaTiO<sub>3</sub>/SrRuO<sub>3</sub> and NdGaO<sub>3</sub>(substrate)/LaSr<sub>0.67</sub>Mn<sub>0.33</sub>O<sub>3</sub>/PbZr<sub>0.2</sub>Ti<sub>0.8</sub>O<sub>3</sub>/LaSr<sub>0.67</sub>Mn<sub>0.33</sub>O<sub>3</sub> were grown by high pressure sputtering and pulsed laser deposition respectively. The BaTiO<sub>3</sub> was deposited as wedge-like films. The thickness gradient was determined by transmission electron microscopy and ranged from approximately 1.5 to 3.5 nm. X-ray diffraction indicated epitaxial and fully strained heterostructures. Tunnel junctions and ferroelectric capacitors were fabricated using optical lithography and ion beam etching. The ferroelectric capacitors showed displacement current down to a thickness of about 2 nm of the BaTiO<sub>3</sub>. Current transport and tunnel magneto resistance were performed down to 10 K and the results will be discussed in the framework of the magneto electric interface effect.

DF 13.5 Wed 16:00 WIL B321

**Conductive atomic force microscopy studies of leakage spot evolution in thin (ZrO<sub>2</sub>)<sub>x</sub>(Al<sub>2</sub>O<sub>3</sub>)<sub>1-x</sub> films.** — •DOMINIK MARTIN<sup>1</sup>, OLIVER BIERWAGEN<sup>2</sup>, MATTHIAS GRUBE<sup>1</sup>, LUTZ GEELHAAR<sup>3</sup>, and HENNING RIECHERT<sup>3</sup> — <sup>1</sup>namlab GmbH, D-01187 Dresden — <sup>2</sup>University of California, Santa Barbara 93106 CA, USA — <sup>3</sup>Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin

In order to achieve at the same time a high dielectric constant and a low leakage current in thin films, an understanding of the charge transport mechanisms is necessary for materials that are inhomogeneous on the nanoscale. Conductive atomic force microscopy (CAFM) measurements on ultrathin (ZrO<sub>2</sub>)<sub>x</sub>(Al<sub>2</sub>O<sub>3</sub>)<sub>1-x</sub> films indicate a strong correlation between leakage spots and crystallites in an otherwise amorphous material. Regular local current-voltage curves were taken at amorphous matrix sites and local current-voltage curves were extracted from multiple images acquired at different biases. The comparison of hysteresis suggests stress induced leakage currents along filamentary leakage paths as well as charge trapping at grain boundaries. The overall local electronic behavior leads to the conclusion that leakage occurs preferably along boundaries between crystallites and the amorphous matrix and that leakage through grain boundaries is comparable to leakage currents through filamentary leakage paths formed by electrical stress.

DF 13.6 Wed 16:20 WIL B321

**Study of C<sub>60</sub> based films formation by NEXAFS** — •DANIEL FRIEDRICH<sup>1</sup>, MARCEL MICHLING<sup>1</sup>, JOLANTA KŁOCEK<sup>1</sup>, DIETER SCHMEISSER<sup>1</sup>, STAS AVDOSHENKO<sup>2</sup>, DMYTRO CHUMAKOV<sup>3</sup>, and EHRENFRIED ZSCHECH<sup>3</sup> — <sup>1</sup>Brandenburgische Technische Universität Cottbus, Angewandte Physik - Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — <sup>2</sup>Department of Chemistry, M. V. Lomonosov Moscow State University, 1 Leninskie Gory, 119991 Moscow, Russian Federation — <sup>3</sup>AMD Fab36 LLC & Co. KG, Wilschdorfer Landstraße 101, 01099 Dresden, Germany

The C<sub>60</sub> fullerenes and some of its -OH, -CF<sub>3</sub> and -Cl derivatives are candidates for application as ultra-low-k insulators in the semiconductor industry. Future preparation of thin films based on these materials requires the stability of the substituted fullerenes against chemical handling and processing steps. The latter issue was addressed by our NEXAFS studies that were done by synchrotron radiation at the beam line U49/2-PGM2 at BESSY II. Performed were the C K-edge NEXAFS studies in total fluorescence and total electron yield modes. The C<sub>60</sub> based films were deposited on silicon by spraying from solutions. The influence of the different substitutional groups with C<sub>60</sub> molecules was studied. The data were compared to the reference spectra of a pure C<sub>60</sub> film. For C<sub>60</sub>(OH)<sub>24</sub>, C<sub>60</sub>-Cl<sub>2</sub> and C<sub>60</sub>(CF<sub>3</sub>)<sub>12</sub> a variance of the intensity of the π\*-resonance as well as shift to higher energies of 0.5 eV (-OH), 0.6 eV (-F), 0.7 eV (-Cl) were observed. The results confirm the necessary stability of the used C<sub>60</sub> derivatives and shall be used for optimization of the film deposition chemistry and conditions.

DF 13.7 Wed 16:40 WIL B321

**Design of nanostructures with maximal magnetoresistance using genetic algorithms** — •DAUNG RUTHAI JARUKANONT — University of Kassel, Kassel, Germany

Spintronics, or spin electronics, involves the study of active control over spin degrees of freedom in solid-state systems. In the field of molecular-electronics, one attempts to make electronic devices using organic molecules. Traditionally these two areas have lived separate lives. Recently experiments have indicated a possible pathway towards their integration. In molecular-spintronics, the spin-polarized currents are carried through molecules, and these can affect the state of the molecule. We study the system of an organic molecule between two ferromagnetic electrodes. The calculations are based on the non-equilibrium Green's function and the Keldysh formalism for the

tight-binding Hamiltonian. We show that organic spin valves can exhibit a bias-dependent magnetoresistance(MR). The magnitude of MR depends on the details of the molecules. These will allow us to suggest an appropriate choice for molecules for molecular-spintronics devices. However since the number of organic molecules that are available is enormous, it is currently very difficult to predict which molecules would be suitable for such devices. We perform a Genetic Algorithm to optimize the magnitude of MR and determine the appropriate molecular choices.

## DF 14: Photonic Dielectrics III

Time: Thursday 10:00–13:00

Location: WIL A317

**Invited Talk** DF 14.1 Thu 10:00 WIL A317

**Spatial nonlinear optics in photonic crystals** — •DETLEF KIP — Institut für Physik und Physikalische Technologien, TU Clausthal

Künstlich strukturierte Materialien, sogenannte Metamaterialien, weisen radikal neue optische Eigenschaften auf. Ein Beispiel sind Halbleiter oder Dielektrika mit einer periodischen Modulation des Brechungsindex, die analog zu kristallinen Festkörpern eine optische Bandstruktur zeigen: Wellenausbreitung in Form von Floquet-Bloch-Moden ist nur in erlaubten Bändern möglich, welche durch Bandgaps voneinander getrennt sind. Für zukünftige, äußerst kompakte photonische Bauelemente, aber auch für das grundlegende Verständnis nichtlinearer periodischer Systeme, ist die Untersuchung der nichtlinearen Wellenausbreitung in photonischen Kristallen von großem Interesse. Modellhaft lassen sich solche nichtlinearen Eigenschaften eindimensionaler photonischer Kristalle in evaneszent gekoppelten Streifenwellenleiterarrays untersuchen, welche sich in Lithiumniobat realisieren lassen. Optisch induzierte Defekte führen hier auf räumlich lokalisierte Zustände oder diskrete Solitonen mit Ausbreitungskonstanten innerhalb der Bandlücke; die Wechselwirkung solcher "Quasiteilchen" lässt sich für zukünftige rein optische Schalter ausnutzen. Daneben erlauben nichtlineare räumlich periodische Strukturen das Studium einer Vielzahl weiterer Wellenphänomene. Beispiele im Vortrag sind räumliche Rabi-Oszillationen in periodisch modulierten Gittern oder die Bildung von räumlichen Frequenzkämmen und Superkontinuum über nichtlineare Vier-Wellen-Mischung von Floquet-Bloch-Moden.

**5 min. break**

DF 14.2 Thu 10:40 WIL A317

**Theoretical discussion of present and novel optical methods for space-charge wave analysis** — •KAY-MICHAEL VOIT, BURGHARD HILLING, and MIRCO IMLAU — Department of Physics, University of Osnabrück, Osnabrück, Germany

Space-charge waves are commonly generated in semi-insulating materials via exposure to an oscillating sinusoidal light interference pattern under an application of high electric fields. However, both the study of nonlinear mutual interactions of SCWs and the investigations of charge-transport properties by SCW spectroscopy are restricted by the assumptions underlying the theoretical concept for SCW analysis: (1) the oscillation amplitudes should be smaller than unity so that the oscillating fringe pattern can be separated into a static and two counterpropagating running gratings and, (2) the modulation depth of the fringe pattern should be smaller than unity. Furthermore, the analysis does not allow to determine the sign of the involved charge carriers. Hence it was the aim of our theoretical and experimental study to develop a new technique which overcomes these restrictions. In this contribution, the assumptions made for the analysis of the oscillating technique are presented and discussed with respect to the experimental restrictions. The novel approach of SCW generation by simultaneous exposure with a static and a running fringe pattern having the same spatial frequency is developed starting from the Kiev equations. Key aspects of the derivation are presented and the formula are compared to the well-known equations for SCW generation with an oscillating fringe pattern.

DF 14.3 Thu 11:00 WIL A317

**Space-charge wave excitation by static and moving interference patterns** — •BURKHARD HILLING, KAY-MICHAEL VOIT, and MIRCO IMLAU — Department of Physics, University of Osnabrück,

Germany

We report on our first experimental results, where SCW excitation was successfully realized by simultaneous exposure with a static and a running interference pattern having the same spatial frequency. The static and running interference patterns are generated independently from each other using a new designed four-beam interferometer with only one light source. For this study, a single crystal of BGO ( $\text{Bi}_{12}\text{GeO}_{20}$ ) was applied as an example. The investigations were performed at a wavelength of 514 nm using a total light intensity of  $30 \text{ mW/cm}^2$  and spatial frequencies of  $(0.5 - 12) \cdot 10^3 \text{ cm}^{-1}$ , while static electric fields of up to  $10 \text{ kV/cm}$  were applied. For a better evaluation of this method SCW were also excited in the same sample under the same experimental conditions using the established method of an oscillating interference pattern. The comparison of both sets of data shows an improvement in the way of excitation of the new method, particularly the quality factor is increased. This method also enables us to determine the sign of the charge carriers participating in SCW formation. Further advantages and disadvantages are discussed. Financial support from the Deutsche Forschungsgemeinschaft within the Graduate College 695 is gratefully acknowledged.

DF 14.4 Thu 11:20 WIL A317

**UV-assisted domain patterning of MgO-doped lithium niobate crystals** — •HENDRIK STEIGERWALD, NIKLAS WAASEM, FABIAN LUEDTKE, and KARSTEN BUSE — Institute of Physics, University of Bonn, Wegelerstrasse 8, 53115 Bonn, Germany

Periodically-poled lithium niobate ( $\text{LiNbO}_3$ ) with domain structures in the micrometer regime is of great relevance, e.g. for nonlinear optics. Efficient frequency conversion in this material is usually hampered by optical damage, i.e., undesired index and absorption changes. MgO-doping increases the optical damage threshold, but makes the poling process more challenging, especially for small domain structures in bulk crystals. We obtain such patterns in MgO-doped near-stoichiometric  $\text{LiNbO}_3$  using structured UV-illumination, which reduces the coercive field for electric field locally. Bulk domain gratings with a period length of  $10 \mu\text{m}$  are realized. Another mechanism that lowers the coercive field strength is heating. We show that for combination of UV-illumination and heating of the crystal both effects add up and the coercive field strength is reduced by a factor of four.

\*Financial support from the Deutsche Telekom AG is gratefully acknowledged.

DF 14.5 Thu 11:40 WIL A317

**Optischer Schaden in Protonenausgetauschten planaren Wellenleitern in Lithiumniobat-Kristallen** — •FABIAN LUEDTKE<sup>1</sup>, JAVIER VILLARROEL<sup>2</sup>, ANGEL GARCÍA-CABAÑES<sup>2</sup>, MERCEDES CARRASCOSA<sup>2</sup> und KARSTEN BUSE<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Bonn, Wegelerstraße 8, 53115 Bonn, Deutschland — <sup>2</sup>Departamento de Física de Materiales C-IV, Universidad Autónoma de Madrid, Campus Cantoblanco, E-28049, Madrid, España

Lithiumniobat-Kristalle sind auf Grund ihrer Ferroelektrizität und ihrer optischen Eigenschaften von großer Bedeutung im Bereich der integrierten und der nichtlinearen Optik. Für Anwendungen bei hohen Lichtintensitäten kann der photorefraktive Effekt zum begrenzenden Faktor werden, in diesem Fall spricht man vom „optischem Schaden“. Für die quantitative Untersuchung dieser lichtinduzierten Brechungsindexänderungen bieten sich interferometrische Verfahren an. Kürzlich wurde ein Mach-Zehnder-Interferometer für die Charakteri-

sierung des optischen Schadens in planaren Wellenleitern vorgestellt. Durch zusätzliche Messungen der Intensitätsschwelle für signifikante Verzerrung des Strahlprofils konnten Brechungsindexänderungen in der Größenordnung  $1 \times 10^{-4}$  als Schwellenwert für eine drastische Verschlechterung des Strahlprofils identifiziert werden. Untersuchungen von Dunkelzerfällen der Brechungsindexänderungen lassen einen Beitrag der Dunkelheitfähigkeit zum optischen Schaden ausschließen.

\*Wir danken der Deutschen Telekom AG für finanzielle Unterstützung.

DF 14.6 Thu 12:00 WIL A317

**Optical cleaning of lithium niobate crystals for suppression of optical damage\*** — ●CARSTEN BECHER<sup>1</sup>, MICHAEL KÖSTERS<sup>1</sup>, DANIEL HAERTLE<sup>1</sup>, BORIS STURMAN<sup>2</sup>, and KARSTEN BUSE<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany — <sup>2</sup>Institute of Automation and Electrometry, Novosibirsk 630090, Russia

Lithium niobate (LiNbO<sub>3</sub>) is a promising material for optical applications, e.g., electro-optic modulation, holography, and frequency conversion. However, the photorefractive effect in its unwanted form, the so-called “optical damage”, still inhibits the use of undoped LiNbO<sub>3</sub> at high light intensities: Light-induced refractive index changes cause deteriorations of the light beam and, e.g., disturb quasi-phase-matching, thus limiting the efficiency of non-linear optical processes. Optical cleaning as a method for suppression of optical damage in congruent, undoped LiNbO<sub>3</sub> crystals is presented: At sufficiently high temperatures, photo-excitabile electrons are removed from an area illuminated by visible light due to the bulk-photovoltaic effect. While at room temperature, an arising electric field would quickly block the photovoltaic drift, at elevated temperatures, H<sup>+</sup>-ions are mobile and can compensate for this electric field. Optical cleaning is studied by two independent methods: Determination of the threshold-intensities for beam fanning, as well as measurements of birefringence changes.

\*Financial support from the Deutsche Forschungsgemeinschaft (FOR 557) and from the Deutsche Telekom AG is gratefully acknowledged.

DF 14.7 Thu 12:20 WIL A317

**Temperature dependent Urbach tail measurements of CaF<sub>2</sub> single crystals** — ●MARTIN LETZ<sup>1</sup>, ALEXANDER GOTTWALD<sup>2</sup>, MATHIAS RICHTER<sup>2</sup>, and LUTZ PARTHIER<sup>3</sup> — <sup>1</sup>Schott AG, Research and Development, D-55014 Mainz — <sup>2</sup>Physikalisch-Technische Bundesanstalt, D-10587 Berlin — <sup>3</sup>Schott Lithotec AG, Otto-Schott Str. 13, D-07745 Jena

In the deep ultra-violet spectral range the transmission of high purity CaF<sub>2</sub> was measured using synchrotron radiation. In the vicinity of the band gap below 11.2 eV or for wavelength longer than 90 nm, a scaling behaviour of the absorption as a function of photon energy was observed. Temperature dependent measurements allow to distinguish different absorption mechanism which differ by their ability to couple to phonon excitations. These two types of Urbach tails were analyzed. The origin of the temperature independent tail is due to defects in the lattice whereas the temperature dependent part originates from short time localization of exciton modes coupling to lattice distortion.

DF 14.8 Thu 12:40 WIL A317

**Study of vacancies and extended defects in SrTiO<sub>3</sub>** — ●M. ZSCHORNAK<sup>1,2</sup>, E. GUTMANN<sup>2</sup>, H. STÖCKER<sup>2</sup>, I. SHAKHVERDOVA<sup>2</sup>, T. WEISSBACH<sup>2</sup>, D.C. MEYER<sup>2</sup>, and S. GEMMING<sup>1</sup> — <sup>1</sup>Institute of Ion Beam Physics and Materials Research, FZ Dresden-Rossendorf, 01328 Dresden, Germany — <sup>2</sup>Institute of Structural Physics, TU-Dresden, 01062 Dresden, Germany

SrTiO<sub>3</sub> is an oxide crystallizing with cubic perovskite-type of structure that exhibits a high tunability of dielectric, electric, mechanical and optical properties by means of defects. Apart from dopants, also intrinsic oxygen vacancies or ordered stacking faults, e.g. Ruddlesden-Popper (RP) phases SrO(SrTiO<sub>3</sub>)<sub>n</sub>, may influence these properties. We have investigated the structural stability, electronic properties and surface energies of such RP phases up to  $n = 5$  by means of density-functional theory. Further, we have theoretically verified an anisotropic reversible elastic softening along an O-deficient (100) direction recently found in nano-indentation of SrTiO<sub>3</sub> under influence of an electric field.

## DF 15: Thin Films and Nanostructures II

Time: Thursday 10:40–13:00

Location: WIL B321

DF 15.1 Thu 10:40 WIL B321

**Interface effects in solid electrolytes** — ●BJÖRN MARTIN and HERBERT KLIEM — Saarland University, Germany

To investigate interface effects, thin films of ion conducting polyethylene oxide (PEO) doped with different salt concentrations are used. Capacitance structures with evaporated Al or Cu electrodes are assembled. An ionic space charge polarization prevails in these systems.

For computer simulations, a three-dimensional discrete hopping model is developed. Negative ions can fluctuate thermally activated over energy barriers in a multiwell potential. The interactions of the ions with the electrodes are considered using the method of images. Also, electrostatic interactions between all ions and between the ions and a positive background charge providing neutrality are considered.

The attractive Coulomb forces between the original charges and the image charges cause a charge accumulation at the electrodes even without applied field as predicted in the simulations. Due to the repulsive forces of these accumulation layers a depletion of mobile charges towards the volume of the sample is found. This charge distribution causes an internal potential with a maximum in the middle of the sample. In the experiment, this potential distribution can be determined using a scanning Kelvin probe which detects the surface potential between the electrodes.

Furthermore, the electrode effects are responsible for the dynamic behavior of the systems like the Kohlrausch behavior of the polarization current and thus the increase of the dielectric permittivity at low frequencies, and the onset of charge injection.

DF 15.2 Thu 11:00 WIL B321

**Characterization of PbSc<sub>0.5</sub>Ta<sub>0.5</sub>O<sub>3</sub> epitaxial thin films prepared by Pulsed Laser Deposition** — ●ANUJ CHOPRA, MARIN ALEXE, BALAJI ISHWARRAO BIRAJDAR, IONELA VREJOIU, and DIETRICH HESSE — Max Planck Institute of Microstructure Physics, Halle, D-06120, Germany

Epitaxial PbSc<sub>0.5</sub>Ta<sub>0.5</sub>O<sub>3</sub> (100) (PST) thin films of thickness 70 nm were deposited on vicinal SrTiO<sub>3</sub> (STO) (100) substrates with a layer of SrRuO<sub>3</sub> (SRO) as a bottom electrode by pulsed laser deposition (PLD) at 823K. Their crystal orientation, topography and microstructure were analysed by X-ray diffraction, atomic force microscopy (AFM) and transmission electron microscopy (TEM), respectively. The films deposited at temperature higher than 823K showed the presence of pyrochlore phase whereas films grown at 823K were perovskites. The in-plane and out-of-plane epitaxial relationships were studied by  $\Phi$  and  $\theta$ - $2\theta$  scans respectively. AFM revealed a smooth surface with RMS of 1.1nm. Superstructure reflections obtained in the TEM diffraction patterns of the films confirm cation ordering. The films were characterized by using polarization vs electric field (P-E) and switching current vs voltage (I-V) measurements. Polarization of the epitaxial films at zero electric field was  $2\mu\text{C}/\text{cm}^2$  at room temperature. Cation ordering with post annealing of the films is still under investigation. This work describes the preparation and characterization of epitaxial films of PST (100) for the first time and indicates PST as a potential candidate for infra-red image sensor applications.

DF 15.3 Thu 11:20 WIL B321

**Switching kinetics in epitaxial BiFeO<sub>3</sub> thin films with different orientations** — ●DANIEL PANTEL<sup>1</sup>, YING-HAO CHU<sup>2</sup>, RAMAMOORTHY RAMESH<sup>3</sup>, and MARIN ALEXE<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany — <sup>2</sup>Department of Materials Science and Engineering, National Chiao Tung University, Hsinchu, Taiwan 30010, R.O.C. — <sup>3</sup>Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA

Due to simultaneously ferroelectric and antiferromagnetic ordering at room temperature multiferroic BiFeO<sub>3</sub> (BFO) is a potential material for magnetoelectric devices. Furthermore, it is a Pb-free ferroelectric with high remnant polarization and therefore a promising candidate for environmental-friendly applications such as non-volatile memories.

For all applications understanding of the detailed switching behavior in BFO is essential.

Large timescale (100 ns to 1 s) voltage pulse trains were used to examine the switching kinetics in BFO thin films with (001), (110) and (111) orientations as a function of applied voltage and time. The kinetics are analyzed in terms of Kolmogorov-Avrami-Ishibashi (KAI) theory and compared with standard systems such as epitaxial  $\text{Pb}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3$  (PZT) films. Likewise in fully c-oriented PZT films, BFO fits well the KAI-model in the high field region, whereas the low field region shows non-KAI kinetics comparable with PZT films with  $90^\circ$  domain walls.

DF 15.4 Thu 11:40 WIL B321

**Stabilization of out-of-plane polarization and head-to-head  $180^\circ$  domain walls in ferroelectric materials** — ●KOUROSH RAHMANIZADEH, GUSTAV BIHLMAYER, and STEFAN BLÜGEL — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Experimental studies suggest that defects play an important role in ferroelectric materials. Employing density functional theory calculations based on the full-potential linearized augmented planewave method as implemented in the FLEUR code ([www.flapw.de](http://www.flapw.de)), we studied the polarization perpendicular to the surface of thin films of the ferroelectric perovskites  $\text{BaTiO}_3$  and  $\text{PbTiO}_3$ . Without an electric field that compensates the depolarization field a polarization perpendicular to the surface is not stable, but we can stabilize an out-of-plane polarization with different types of defects at the surface. This mechanism can also be at work at head-to-head and tail-to-tail  $180^\circ$  domain walls, which can occur in these compounds. Although nominally a substantial extra charge is present at these surfaces or interfaces, the electronic properties are found to be very similar to the bulk of the perovskites.

DF 15.5 Thu 12:00 WIL B321

**Study of polyimide after graphitization with low-energy  $\text{Ar}^+$  ion irradiation by NEXAFS** — ●MARCEL MICHLING<sup>1</sup>, DANIEL FRIEDRICH<sup>1</sup>, DIETER SCHMEISSER<sup>1</sup>, YURI KOVAL<sup>2</sup>, and PAUL MÜLLER<sup>2</sup> — <sup>1</sup>Brandenburgische Technische Universität Cottbus, Angewandte Physik/Sensorik, K.- Wachsmann-Allee 1, 03046 Cottbus — <sup>2</sup>Universität Erlangen Nürnberg, Experimental Physik/Supraleitung, Erwin-Rommel-Str. 1, 91058 Erlangen

In this contribution we report on investigations of the electronic structure of  $\text{Ar}^+$  irradiated polyimide samples by using NEXAFS. The NEXAFS measurements were done at the U49/2-PGM2 beam line of BESSY II, Berlin using TEY and TFY detection.

Polyimide samples are prepared using low  $\text{Ar}^+$  dose while the temperature of the samples is varied between 300K and 700K. In the NEXAFS data at the Carbon K-edge we see substantial changes between differ-

ent samples. The differences appear in particular in the more surface sensitive TEY-Signal.

The NEXAFS data are consistent with the graphitization of the surface upon  $\text{Ar}^+$  bombardment as we identify the characteristic absorption bands of graphitic carbon. Its relative content increases with increasing sample temperature. In contrast, in the more bulk sensitive TFY data, the emission characteristic of polyimide is maintained.

The possibility to cover insulating polymers with a conducting layer is a great demand for many applications. Because of the relative low price of the basic materials, the irradiation with low-energy ions will play an important role in the microelectronics of the future.

DF 15.6 Thu 12:20 WIL B321

**Effects of rare earth manganite on structural, magnetic and ferroelectric properties of  $\text{BiFeO}_3$  thin films** — ●ABDELLILAH LAHMAR, SALAH HABOUTI, MATTHIAS DIETZE, CLAUS-HENNING SOLTERBECK, and MOHAMMED ES-SOUNI — Institute for Materials and Surface Technology, University of Applied Sciences Kiel, Germany

The results of structural studies of pure-phase perovskite thin films of  $\text{BiFeO}_3 - 10\% \text{RMnO}_3$  ( $R = \text{La, Eu, Gd, Tb}$  and  $\text{Dy}$ ) are presented. Raman Scattering studies show lines broadening similar to what is reported for  $\text{RMnO}_3$ ; they were attributed to Jahn-Teller distortion and orthorhombic structural change. Evidence of an anomaly of the orthorhombic distortion at  $\text{GdMnO}_3$  could be obtained. Interestingly the addition of  $\text{GdMnO}_3$  leads to a substantial increase in magnetization, combined with moderate ferroelectric polarization. All other compositions are characterized by higher ferroelectric polarization but almost no magnetization.

DF 15.7 Thu 12:40 WIL B321

**Growth of Conductive  $\text{HfO}_{2-x}$  Thin Films by Reactive Molecular Beam Epitaxy** — ●ERWIN HILDEBRANDT<sup>1</sup>, JOSE KURIAN<sup>1</sup>, HANS-JOACHIM KLEEBE<sup>2</sup>, and LAMBERT ALFF<sup>1</sup> — <sup>1</sup>Institut für Materialwissenschaft, TU Darmstadt, Germany — <sup>2</sup>Institut für Angewandte Geowissenschaften, TU Darmstadt, Germany

Thin films of oxygen deficient hafnium oxide were grown on single crystal *c*-cut and *r*-cut sapphire substrates by reactive molecular beam epitaxy. The oxidation conditions during growth were varied within a wide range using RF-activated oxygen. Hafnium oxide thin films were characterized using X-ray diffraction, resistivity measurements ( $\rho$ -T) and transmission electron microscopy (TEM). The results show a dramatic increase in conductivity of the deposited oxygen deficient hafnium oxide thin films with decreasing oxidation conditions during growth. The electrical properties of deficient hafnium oxide thin films varied from insulating over semiconducting to conducting. X-ray diffraction data as well as TEM data rule out the possibility of conductivity due to metallic hafnium.

## DF 16: Thin Films and Nanostructures III

Time: Thursday 14:30–16:30

Location: WIL B321

### Invited Talk

DF 16.1 Thu 14:30 WIL B321

**Simulation of Defects and Domain Structures in Ferroelectrics** — ●RALF MÜLLER — Department of Civil Engineering and Geodesy, Solid Mechanics, TU Darmstadt, Hochschulstr. 1, 64289 Darmstadt, Germany

The macroscopic material properties of ferroelectric materials strongly depend on their complex microstructure, which includes length scales from the atomistic level up to the grain size level. Crucial for the understanding of fatigue, degradation and aging phenomena is the interaction of domain walls and domain structures with various defects in the material. In order to analyse these interactions a thermodynamically consistent continuum mechanical approach is taken. Domain walls are modelled as sharp interfaces or are simulated by a phase field approach. The phase field approach can be understood as a regularization of the sharp interface model. Both models are implemented into a special finite element method. Techniques to incorporate localized defects in the continuum are discussed, by a comparative study between atomistic and continuum mechanical simulations. Additionally, the interaction between defects can be studied using thermodynamic arguments.

Pinning phenomena of domain walls at electrode and point defects are shown. Macroscopic material properties are derived from simu-

lations with evolving microstructures by homogenization procedures. The simulated material behavior is compared to some of the few multi-axial experiments available in the literature.

### 5 min. break

DF 16.2 Thu 15:10 WIL B321

**Optische und strukturelle Untersuchung an Bariumtitanat-Dünnschichten** — ●STEFAN SCHÖCHE, RÜDIGER SCHMIDT-GRUND, CHRIS STURM, HOLGER HOCHMUTH, MATTHIAS BRANDT, MICHAEL LORENZ und MARIUS GRUNDMANN — Fakultät für Physik und Geowissenschaften, Institut für experimentelle Physik II, Universität Leipzig

Aufgrund diverser Anwendungsmöglichkeiten in Elektronik, Elektromechanik und Elektrooptik sind ferroelektrische Oxide zentraler Bestandteil aktueller Forschung. Insbesondere für optische Anwendungen, ist eine genaue Kenntnis der dielektrischen Funktion (DF) über einen weiten Spektralbereich erforderlich.

Wir präsentieren eine detaillierte Untersuchung der DF epitaktischer  $\text{BaTiO}_3$  (BTO)-Dünnschichten, abgeschieden auf (100)-, (110)- und (111)-orientierten  $\text{SrTiO}_3$  (STO)-Substraten mittels gepulster Laserablation (PLD). Es wurden spektroskopische Ellipsometrie-Messungen im Spektralbereich 0.03 – 0.4 eV bzw. 0.8 – 5 eV durchgeführt und mit

Ergebnissen von struktursensitiven Messmethoden wie Rasterkraftmikroskopie und Röntgenbeugung korreliert.

Zur Analyse der Ellipsometriedaten wurde ein Schichtstapel-Modell erstellt, bestehend aus parametrisierten DF des STO-Substrats, der BTO-Schicht und einer Oberflächenschicht. Daraus wurden Eigenschaften der Band-Band-Übergänge im Bereich der fundamentalen Bandlücke und höherer kritischer Punkte, sowie Phononenmoden erstmalig für dünne Schichten abgeleitet.

DF 16.3 Thu 15:30 WIL B321

**The Local Field Method for Dielectric Nanocomposites** —  
•MARKUS KÜHN and HERBERT KLIEM — Saarland University, Germany

We focus on nanodielectrics consisting of two different phases. The systems are embedded between coplanar conducting electrodes which are taken into account by the method of image dipoles. Binary mixtures are modelled by neutral atoms with polarizabilities  $\alpha$  and  $\beta$ , respectively. The different atoms are statistically arranged on cubic lattice sites. For different volume ratios and different dielectric contrasts of the two phases the dipole moments and local fields are calculated. For vanishing  $\alpha$ - or rather  $\beta$ -phase the corresponding Lorentz fields are obtained, respectively. The simulation results are compared to the common Maxwell-Garnett mixing rule. In contrast to the local field method which also inherently takes into account all depolarization effects, macroscopic mixing rules are based on a homogenization of heterogeneous systems. This simplified description of the dielectric neglects the real microstructure and the varying local fields. In addition, we investigated two-dimensional nanodielectrics where we have a polar inclusion modelled by permanent bidirectional dipoles at cubic lattice sites. The shape of the inclusion is random and it is surrounded by a matrix of induced dipoles placed at cubic lattice sites. Again, the local field method yields the locally varying dipole moments due to the microstructure.

DF 16.4 Thu 15:50 WIL B321

**Impact of high interface density on ferroelectric and structural properties of  $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  /  $\text{PbZr}_{0.4}\text{Ti}_{0.6}\text{O}_3$  epitaxial multilayers** — •LUDWIG FEIGL<sup>1</sup>, SHIJIAN ZHENG<sup>2</sup>, BALAJI I. BIRAJDAR<sup>1</sup>, BRIAN J. RODRIGUEZ<sup>1</sup>, YINLIAN ZHU<sup>1,2</sup>, MARIN ALEXE<sup>1</sup>, and DIETRICH HESSE<sup>1</sup> — <sup>1</sup>Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — <sup>2</sup>Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese

Academy of Sciences, 72 Wenhua Road, 110016 Shenyang, China

Multilayers consisting of the two tetragonal compositions  $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  and  $\text{PbZr}_{0.4}\text{Ti}_{0.6}\text{O}_3$  were deposited onto a  $\text{SrRuO}_3$  electrode grown on a vicinal (100)  $\text{SrTiO}_3$  substrate. It has been shown by extensive structural investigations comprising transmission electron microscopy in conventional and high resolution mode, reciprocal space mapping and piezoresponse force microscopy that with decreasing layer thickness a transition from a-domains confined to individual layers to a-domains propagating through the whole film takes place. This is caused by the formation of a common strain state of all layers which is responsible for the observed enhancement of the electrical properties. These show a maximum in the product of remanent polarization and dielectric constant at a certain density of interfaces. If the interface density becomes too high the lattice distortion accompanying each interface deteriorates the properties of the multilayer structure.

DF 16.5 Thu 16:10 WIL B321

**Nonlinear Frequency Response of Metal/Ferroelectric/Metal and Metal/Ferroelectric/Semiconductor Heterostructures** —  
•KAY BARZ, MARTIN DIESTELHORST, and HORST BEIGE — Martin Luther-Universität Halle-Wittenberg

By investigating the dynamic behavior of a ferroelectric-semiconductor heterostructure we observed a torus doubling bifurcation together with other interesting frequency responses obviously driven by the nonlinear nature of the sample.[1] In the talk, some of these experimental findings will be presented, mainly focusing on the amplitude-frequency-characteristics observed at different structure types (metal/ferroelectric/metal (MFM) and metal/ferroelectric/semiconductor (MFS)). Concerning the MFS heterostructures it was to clarify, whether the observed nonlinear phenomena can be attributed to the ferroelectric thin film or the semiconductor substrate or if it is an emergent property (i.e. spontaneously arising owing to the system's complexity). Therefore the behavior of the MFS structures was compared to simple MOS-capacitors (metal/oxide/semiconductor). The results on MFM structures show, how hysteresis and its transient alterations due to fatigue manifest in the frequency response. It turns out that ferroelectric thin films and ferroelectric/semiconductor heterostructures provide easy experimental access to interesting phenomena known from theory of nonlinear dynamics.

[1] M. Diestelhorst et.al.; *Phil. Trans. Roy. Soc. A*; 366; 437-446; 2008.