

## 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-Tc 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. Hugschmidt 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.

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DF 2.6 Mon 12:20 WIL A317

**k-space spectroscopy on calcium barium niobate single crystals** — ●URS HEINE<sup>1</sup>, UWE VOELKER<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.