

## Crystallography Division Fachgruppe Kristallographie (KR)

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### Overview of Invited Talks and Sessions

(Lecture room H26; Poster E)

#### Sessions

KR 1.1–1.3	Wed	18:00–20:00	Poster E	<b>Poster</b>
KR 2.1–2.8	Thu	9:30–12:30	H26	<b>Nano- and microstructured dielectrics / thin films (DF, KR)</b>
KR 3.1–3.2	Thu	15:00–15:40	H26	<b>Ceramics and Applications (DF, KR)</b>
KR 4.1–4.4	Thu	15:40–17:00	H26	<b>Crystallography in Materials Science (KR, DF, MI)</b>
KR 5	Thu	17:20–18:00	H26	<b>Mitgliederversammlung der FG Kristallographie</b>

#### Annual General Meeting of the Crystallography Division

Donnerstag, 10.03.2016 17:20–18:00 Raum H26

- Bericht der FG-Leiterin
- Wahl der neuen Leitung
- Verschiedenes

## KR 1: Poster

Time: Wednesday 18:00–20:00

Location: Poster E

## KR 1.1 Wed 18:00 Poster E

**Mechanism of delafossite (CuFeO<sub>2</sub>) formation in aqueous solution** — ●MELANIE JOHN<sup>1</sup>, ALADIN ULLRICH<sup>2</sup>, and SORAYA HEUSS-ASSBICHLER<sup>1</sup> — <sup>1</sup>Ludwig-Maximilians-Universität München, München, Deutschland — <sup>2</sup>Universität Augsburg, Augsburg, Deutschland

Recently we successfully synthesized delafossite (CuFeO<sub>2</sub>) nanoparticles at 70°C by a facile precipitation and ageing process for the first time. In literature, there are only very few references on the formation mechanism of delafossite in aqueous solution. However, for further optimization of the synthesis processes and the transferability to other ABO<sub>2</sub> structures, it is necessary to get a better understanding of the formation mechanisms in this system. Our results show that green rust II (GR-SO<sub>4</sub>, a Fe(II-III) layered double hydroxysulphate) and Cu<sub>2</sub>O precipitate first. During further OH-supply GR-SO<sub>4</sub> oxidizes and forms Fe<sub>10</sub>O<sub>14</sub>(OH)<sub>2</sub>, Cu<sub>2</sub>O and CuFeO<sub>2</sub> crystals. Due to an alkaline pH further CuFeO<sub>2</sub> crystals grow at the cost of the unstable intermediate products. The reaction rate increases with increasing ageing temperature, reaction pH and, in particular, NaOH concentration in the solution. As a result, high crystalline CuFeO<sub>2</sub> nanoparticles showing hexagonal, platy morphology form. The precipitation residues were analyzed using ICP-OES, FTIR, XRD, SEM and TEM.

## KR 1.2 Wed 18:00 Poster E

**Compositional influence on the pyroelectric coefficient of (1-x)PMN-xPT** — ●SVEN JACHALKE, ERIK MEHNER, HARTMUT STÖCKER, ERIK SCHLEICHER, TILMANN LEISEGANG, and DIRK C. MEYER — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Str. 23, 09596 Freiberg

Solid solutions of lead magnesium niobate – Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>, PMN – and lead titanate – PbTiO<sub>3</sub>, PT – in different compositions – (1-x)PMN-xPT – attract a large scientific interest due to their superb electromechanical and electrothermal properties, especially near

the morphotropic phase boundary around  $x = 0.30$ . The present study focuses on the pyroelectric properties, i.e. the change of spontaneous polarization due to temperature fluctuations. Pyroelectric coefficients  $p(T)$  of single crystals are determined systematically with respect to different compositions ( $x = 0.25$  to  $x = 0.32$ ) and crystallographic orientations ( $\langle 111 \rangle$ ,  $\langle 011 \rangle$  and  $\langle 001 \rangle$ ), including ferroelectric-to-ferroelectric and ferroelectric-to-dielectric phase transitions (at the Curie temperature  $T_C$ ), in the temperature range of 273 K to 423 K. Data acquisition and analysis using the Sharp-Garn-method [1] allow separating the pyroelectric from disturbing non-pyroelectric current signals and yield temperature dependent pyroelectric coefficients (accuracy 1–5 %) and polarization.

[1] L. E. Garn and E. J. Sharp, "Use of low-frequency sinusoidal temperature waves to separate pyroelectric currents from nonpyroelectric currents", J. Appl. Phys., Vol. 53, No. 12, p. 8974, 1982.

## KR 1.3 Wed 18:00 Poster E

**Theoretical Exploration of Phase Diagrams using Monte-Carlo Site Swapping** — ●KATHRYN BRADLEY, MATTHEW DYER, JOHN CLARIDGE, GEORGE DARLING, and MATTHEW ROSSEINSKY — Department of Chemistry, University of Liverpool, Crown Street, Liverpool, L69 7ZD, United Kingdom

A method has been developed for investigating the phase diagrams of structures with similar structural motifs, using a combination of structural prediction, forcefield calculations and density functional theory (DFT). Li<sub>3</sub>PO<sub>4</sub> and Li<sub>4</sub>SiO<sub>4</sub> can be described in terms of close-packed oxide lattices with cations present in the interstitial sites. It is therefore possible to generate a superlattice with a mixed composition. The structure is first evaluated using forcefield optimisation with Monte-Carlo site swapping, and the stability of the suggested composition is then assessed using DFT energies. This new approach will help with the exploration of phase diagrams to assist in the field of materials discovery.

## KR 2: Nano- and microstructured dielectrics / thin films (DF, KR)

Time: Thursday 9:30–12:30

Location: H26

## KR 2.1 Thu 9:30 H26

**Fabrication of periodically patterned domain structures in x-cut thin film LiNbO<sub>3</sub>** — PETER MACKWITZ<sup>1</sup>, MICHAEL RÜSING<sup>1</sup>, GERHARD BERTH<sup>1,2</sup>, and ●ARTUR ZRENNER<sup>1,2</sup> — <sup>1</sup>Department Physik, Universität Paderborn, 33098 Paderborn, Germany — <sup>2</sup>Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Within the field of nonlinear optics LiNbO<sub>3</sub> represents an important material with outstanding nonlinear optical properties. It is possible to achieve a highly efficient frequency conversion in LiNbO<sub>3</sub> with periodic poled structures which preserve the quasi phase matching condition. Bulk LiNbO<sub>3</sub> represents one of the major materials for frequency conversion with periodically poled pattern. Concerning the different scattering geometries of LiNbO<sub>3</sub> x-cut samples offer favorable properties regarding the fabrication of periodically pattern and the frequency conversion. For example the most intense tensor element  $d_{33}$  can directly be triggered. Scores of previous works [1] have shown the fabrication and application of periodically poled domain pattern in bulk LiNbO<sub>3</sub>. In this work we have processed x-cut thin film LiNbO<sub>3</sub> samples in order to create a periodically poled pattern. The transferred domain structures were studied with nonlinear microscopy. Concerning the nonlinear measurements the domain structures could clearly be resolved and the poling process was successful. These results hint to the possibility of homogeneous poled domains allowing novel applications in the framework of photonics and integrated optics. [1] L. Gui, H. Hu et al., Opt. Exp. 17, 3923 (2009)

## KR 2.2 Thu 9:50 H26

**Nanostructuring of dielectric surfaces using nanosecond laser radiation assisted by metallic absorber layer** — ●PIERRE LORENZ<sup>1</sup>, MICHAEL KLÖPPEL<sup>1,2</sup>, CHRISTOPH GRÜNER<sup>1</sup>, FRANK FROST<sup>1</sup>, JOACHIM ZAJADACZ<sup>1</sup>, MARTIN EHRHARDT<sup>1</sup>, and KLAUS

ZIMMER<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany — <sup>2</sup>Institute of Scientific Computing, Department of Mathematics, TU Dresden, 01062 Dresden, Germany

The laser-induced structuring of different dielectrics assisted by self-organisation of a molten thin metal layer during laser heating with a 248 nm, 25 ns KrF excimer laser was studied. The nanopattern formation at low laser fluence is caused by instabilities of thin molten metal layer on dielectric surfaces within the laser pulse driven by the surface tension of the liquid metal layer. As dielectric substrate and metallic absorber film SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, and diamond as well as Cr and Mo were used, respectively. Homogenous and pre-structured metal film were irradiated and specific features of the self-organization process found. For instance, the high laser fluence irradiation of the pre-structured films can result in forming different structures. The resultant structures of the film or in the substrate were investigated by atomic force (AFM) and scanning electron microscopy (SEM). These laser-induced nanostructures were imaged by SEM after cross sectioning by focussed ion beam (FIB). The hole-forming process was simulated using a heat equation to describe the laser-heating of the solid and a kind of Navier-Stokes equation to describe the mass transport in the liquid.

## KR 2.3 Thu 10:10 H26

**Production yield of rare-earth ions implanted into an optical crystal** — ●THOMAS KORNER<sup>1</sup>, KANGWEI XIA<sup>1</sup>, ROMAN KOLESOV<sup>1</sup>, NADEZHDA KUKHARCHYK<sup>2</sup>, HANS-WERNER BECKER<sup>3</sup>, BRUNO VILLA<sup>1</sup>, ROLF REUTER<sup>1</sup>, ANDREAS D. WIECK<sup>2</sup>, and JÖRG WRACHTRUP<sup>1</sup> — <sup>1</sup>3. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — <sup>2</sup>Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — <sup>3</sup>RUBION, Ruhr-Universität Bochum, 44780 Bochum, Germany

Rare-earth (RE) ions doped into desired locations of optical crystals might enable a range of novel integrated photonic devices for quantum applications. With this aim, we have investigated the production yield of cerium and praseodymium by means of ion implantation. As a measure, the collected fluorescence intensity from both, implanted samples and single centers was used. With a tailored annealing procedure for cerium, a yield up to 53% was estimated. Praseodymium yield amounts up to 91%. Such high implantation yield indicates a feasibility of creation of nanopatterned rare-earth doping and suggests strong potential of RE species for on-chip photonic devices. Additionally, the potential of evanescently coupling RE ions in YAG to photonic structures is investigated.

KR 2.4 Thu 10:30 H26

**Circular dichroism of the distorted Gyroid photonic crystal** — ●JOHANNES HIELSCHER<sup>1</sup>, SEBASTIAN C. KAPFER<sup>1</sup>, CAROLINE POUYA<sup>2</sup>, PETER VUKUSIC<sup>2</sup>, and GERD E. SCHRÖDER-TURK<sup>3</sup> — <sup>1</sup>FAU Erlangen-Nürnberg, Institut für Theoretische Physik — <sup>2</sup>University of Exeter, School of Physics — <sup>3</sup>Murdoch University, School of Engineering & IT, Maths & Stats

The single Gyroid is a bi-continuous triply-periodic network with chiral  $I_{41}32$  cubic symmetry. When realised with two phases of dielectric contrast, it acts as a photonic crystal. As a such, it has been found in butterfly wings. Due to its chirality, it exhibits circular dichroism in reflectance.

We show that the introduction of a long-wavelength variation of the lattice constant (“sinusoidal chirp”) tunes the coupling of light waves at the interface of the photonic crystal differently depending on circular polarisation, i. e. changes the circular dichroism [1]. Reflectance spectra are gathered from numerical electrodynamics simulations, and are in good agreement with microwave optics measurements on selected 3D-printed replicas. Studying model systems, as the tetragonally distorted Gyroid and its photonic band structure, contributes to our understanding of the intricate geometrical contributions on the reflectance properties of photonic crystals, beyond the unit-cell scale.

[1] J. Hielscher; C. Pouya; P. Vukusic & G. E. Schröder-Turk: Harmonic long-range distortions of Gyroid photonic materials enhance circular dichroism. *In preparation, 2016*

KR 2.5 Thu 10:50 H26

**Flexible formation of coupled active polymeric whispering gallery mode cavities on an elastomer substrate** — ●STEFAN SCHIERLE<sup>1</sup>, TOBIAS SIEGLE<sup>1</sup>, SARAH KRÄMMER<sup>1</sup>, BENJAMIN RICHTER<sup>2</sup>, SENTAYEHU WONDIMU<sup>3</sup>, PETER SCHUCH<sup>3</sup>, CHRISTIAN KOOS<sup>4</sup>, and HEINZ KALT<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — <sup>2</sup>Zoological Institute, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — <sup>3</sup>Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — <sup>4</sup>Institute of Photonics and Quantum Electronics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Optical modes in whispering gallery resonators are classified in analogy to electronic orbitals in atoms. Coupling between multiple resonators allows a photon exchange among them and leads to the formation of so-called photonic molecules.

Dye (pyromethene 597)-doped active micro disk and goblet cavities are structured in a linear configuration by direct laser writing on a flexible elastomer substrate. Stretching the substrate and using its lateral contraction allows a fine tuning of the inter-cavity gaps. This enables the formation of photonic molecules consisting of two and three micro cavities. Spatially resolved spectroscopy demonstrated both the localization of super-modes, e.g. modes being resonant in the coupled system, and also the extinction of non-resonant modes in the photonic molecules. Relaxation of the substrate shows a change back to the uncoupled modal spectrum.

20 min. break

KR 2.6 Thu 11:30 H26

**Electrospun dye-doped polymeric fiber networks for alcohol vapor detection** — ●SARAH KRÄMMER<sup>1</sup>, FABRICE LAYE<sup>1</sup>, CHRISTOPH VANNAHME<sup>2</sup>, MINH TRAN<sup>1</sup>, PASCAL KIEFER<sup>1</sup>, FELIX FRIEDRICH<sup>1</sup>, CAMERON L. C. SMITH<sup>2</sup>, ANA C. MENDES<sup>3</sup>, IOANNIS S. CHRONAKIS<sup>3</sup>, ANDERS KRISTENSEN<sup>2</sup>, and HEINZ KALT<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — <sup>2</sup>Department of Micro- and Nanotechnology, Technical University of Denmark (DTU), 2800 Kgs., Lyngby, Denmark — <sup>3</sup>Nano-BioScience Research Group, DTU-Food, Technical University of Denmark (DTU), 2800 Kgs., Lyngby, Denmark

Recently we have shown that random resonators within dye-doped electrospun polymeric fiber networks lead to lasing emission [1]. Here, we demonstrate that the narrow laser emission lines can be used as sensor signal. When the fiber networks are exposed to alcohol vapors, the alcohol molecules diffuse into the polymer and cause swelling of the fibers. This swelling process changes the effective refractive index of the fiber resonator and thus causes a spectral shift of the laser mode. In various sensing experiments we analyzed the spectral shift of the lasing modes for different concentrations of ethanol and methanol. For the investigated concentration range we found a linear dependency of the shift on the alcohol concentration. The time resolved signal reveals different saturation times for the different alcohols which are related to the different diffusion constants and allow a differentiation of ethanol and methanol.

[1] Krämmmer et al., Adv. Mater., 26, 8096-8100, 2014

KR 2.7 Thu 11:50 H26

**Implanted Strontium Titanate Single Crystals for Energy Storage Applications** — ●MAX STÖBER<sup>1</sup>, CHARAF CHERKOUK<sup>1</sup>, JULIANE WALTER<sup>1</sup>, MATTHIAS SCHELTER<sup>2</sup>, JENS ZOSEL<sup>2</sup>, RALPH STROHMEYER<sup>1</sup>, SLAWOMIR PRUCNAL<sup>3</sup>, TILMANN LEISEGANG<sup>1</sup>, and DIRK CARL MEYER<sup>1</sup> — <sup>1</sup>TU Bergakademie Freiberg — <sup>2</sup>Kurt Schwabe Institute Meinsberg — <sup>3</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf,

A rapid increase of the demand on efficient energy storage solutions requires new approaches beyond the Li-ion technology. In particular, metal-air batteries as well as solid-state fuel cells offer a great potential for high-energy-density storage devices. Since the efficiency of such devices is significantly limited by the activation of both the oxygen reduction reaction (ORR) and the ionic and electronic conductivities, an adequate porosity as well as a controlled doping are required. The ion implantation is a key technology to achieve this goal. In this work, p- and n-doped strontium titanate (SrTiO<sub>3</sub>) single crystals were used as oxidic materials. The oxygen exchange kinetics as well as the structural changes of the SrTiO<sub>3</sub> crystal surface induced by the ion implantation were investigated. On one hand, the depth profile of dopant concentration and dopant valence state were determined using sputtered X-ray photoelectron spectroscopy (XPS). On the other hand, the overall oxygen exchange kinetic of the implanted SrTiO<sub>3</sub> crystal was quantitatively described by means of coulometric titration using Zirox system (ZIROX GmbH, Germany). Furthermore, the surface morphology of the samples was investigated using atomic force microscopy (AFM).

KR 2.8 Thu 12:10 H26

**Die wahre Definition der Lichtgeschwindigkeit** — ●ADOLF BALITZKA — 88682 Salem Baden, Alpenblick 6

Der Vortrag beschreibt den mathematischen Weg vom Cosinusquadrat des sog. "Magic Angle" bzw. "Zauberwinkel" (1/3) zur Lichtgeschwindigkeit. Bekanntlich spielt dieser Winkel bei Versuchen mit magnetischen Momenten eines Festkörpers eine wichtige Rolle.

### KR 3: Ceramics and Applications (DF, KR)

Time: Thursday 15:00–15:40

Location: H26

KR 3.1 Thu 15:00 H26

**Crystallization in luminescent borate glass for use in white LEDs** — ●A. CHARLOTTE RIMBACH<sup>1</sup>, FRANZISKA STEUDEL<sup>2</sup>, and STEFAN SCHWEIZER<sup>1,2</sup> — <sup>1</sup>South Westphalia University of Applied

Sciences, Luebecker Ring 2, 59494 Soest — <sup>2</sup>Fraunhofer Application Center for Inorganic Phosphors, Branch Lab of Fraunhofer Institute for Microstructure of Materials and Systems IMWS, Luebecker Ring 2, 59494 Soest

The majority of white LEDs is comprised of a blue light emitting diode and a yellow phosphor. The phosphor powder, which converts a part of the blue light to yellow light, is embedded in an organic polymer and directly coated onto the LED chip. Heat-induced degradation of the polymer-based encapsulate, however, results in an efficiency decrease and color temperature change. Luminescent glasses and glass ceramics might represent an interesting alternative due to their higher thermal and chemical stability. For optical activation, the glasses are doped with rare-earth ions such as europium and terbium. Due to the relatively low absorption coefficient of the rare-earths the blue LED light is only absorbed by a small amount resulting in a too high color temperature. To increase the optical absorption by multiple scattering and reflection the glasses are subsequently processed to glass ceramics. This work focuses on the crystallization process in europium-doped lithium-aluminium-borate glass upon annealing at different temperatures for different periods of time. Differential scanning calorimetry and X-ray diffraction are the methods chosen to monitor the crystal growth and to identify the crystal phases.

KR 3.2 Thu 15:20 H26

Small-scale Dislocation Plasticity in Strontium Titanate —

•ALEXANDER STUKOWSKI, FARHAN JAVAID, KARSTEN DURST, and KARSTEN ALBE — Technische Universität Darmstadt

Strontium titanate (STO) is an optically transparent perovskite oxide ceramic material. In contrast to other ceramics, single crystal STO plastically deforms under ambient condition, without showing a phase transition or early fracture. This remarkable ductility makes it a prime candidate for different technological applications. However, while the mechanical behavior of bulk STO has been studied extensively using uniaxial compression testing techniques, little is known about the local, small-scale behavior and the details of dislocation-based nanoplasticity in this perovskite material.

In this contribution we compare results obtained from new nanoindentation experiments and corresponding large-scale molecular dynamics simulations. The evolution of the plastic zone and dislocation structures that form underneath the indenter is investigated using etch-pit methods in experiments and a novel three-dimensional defect identification technique in atomistic computer models. The latter allows tracing the evolution of the complete dislocation line network as function of indentation depth, quantifying the activity of different slip systems, and correlating this information with the recorded load-displacement curves and hardness data.

## KR 4: Crystallography in Materials Science (KR, DF, MI)

Time: Thursday 15:40–17:00

Location: H26

KR 4.1 Thu 15:40 H26

**Low temperature synthesis of CuFeO<sub>2</sub> (delafossite) between 50°C and 90°C: A new process solely by precipitation and ageing** — •MELANIE JOHN<sup>1</sup>, ALADIN ULLRICH<sup>2</sup>, and SORAYA HEUSS-ASSBICHLER<sup>1</sup> — <sup>1</sup>Ludwig-Maximilians-Universität München, München, Deutschland — <sup>2</sup>Universität Augsburg, Augsburg, Deutschland

Due to the large variability of technical applications of delafossite compounds e.g. as a catalyst, in p-type conduction oxides or as a cathode in Li-ion batteries, the synthesis of ABO<sub>2</sub> structures have received much attention the last years. Delafossite syntheses have been reported via solid state reaction and sol-gel processes using high temperatures between 900-1200°C or hydrothermal synthesis methods using at least autogenous pressure so far. We now synthesized CuFeO<sub>2</sub> nanoparticles, the parent mineral of the Delafossite group, solely by precipitation and subsequent ageing at temperatures between 50°C and 90°C and without any additives controlling the oxidation state of copper for the first time. With this method, it is possible to synthesize a mixture of 2H (space group (SG): P6<sub>3</sub>/mmc) and 3R polytype (SG: R-3m) of delafossite showing hexagonal morphology within 10 hours. The experimental conditions regulate the phase assemblage, size and the necessary ageing time. The synthesized material was analyzed by ICP-OES, FTIR, XRD, SEM, TEM and magnetic measurements.

KR 4.2 Thu 16:00 H26

**Investigation of the sodium solid electrolyte Na<sub>5</sub>YSi<sub>4</sub>O<sub>12</sub>** — •WOLFRAM MÜNCHGESANG<sup>1</sup>, ANASTASIA VYALIKH<sup>1</sup>, FALK MEUTZNER<sup>1</sup>, TINA NESTLER<sup>1</sup>, DÖRTE WAGNER<sup>2</sup>, AXEL ROST<sup>2</sup>, ULRIKE LANGKLOTZ<sup>2</sup>, JOCHEN SCHILM<sup>2</sup>, TILMANN LEISEGANG<sup>1</sup>, and DIRK C. MEYER<sup>1</sup> — <sup>1</sup>Technische Universität Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg, Germany — <sup>2</sup>Fraunhofer Institute für Ceramic Technologies and Systems IKTS, Winterbergstraße 28, 01277 Dresden, Germany

Beside the well-known sodium solid electrolytes  $\beta$ -Alumina and NASICON, Na<sub>5</sub>YSi<sub>4</sub>O<sub>12</sub> (NYS) is another promising crystal structure with a high ionic conductivity. Its main advantage over the two above-mentioned structures is the reduced production complexity and the associated costs. However, very little is known about its complex crystal structure and properties. Starting from a crystallographic point of view, sodium ion conduction pathways have been considered with the Voronoi-Dirichlet and the energy-scaled bond valence approaches, and compared with the pathways in other ion conductors.

In the present work, the crystal structure and ionic conductivity in polycrystalline NYS-materials, obtained by a glass-ceramic process, has been analysed using solid-state NMR and Electrical Impedance Spectroscopy respectively, and interpreted in respect to the theoretical predictions.

This work was financed by the BMWi within the project BaSta (0325563D) and the BMBF within the project SyNeSteSia (05K2014).

KR 4.3 Thu 16:20 H26

**Measuring electron-phonon coupling by RIXS: the showcase of anatase TiO<sub>2</sub>** — •SIMON MOSER<sup>1</sup>, SARA FATALE<sup>1</sup>, PETER KRÜGER<sup>2</sup>, HELMUTH BERGER<sup>1</sup>, PHILIPPE BUGNON<sup>1</sup>, ARNAUD MAGREZ<sup>1</sup>, HIDEHARU NIWA<sup>3,4</sup>, JUN MIYAWAKI<sup>3,4</sup>, YOSHIHISA HARADA<sup>3,4</sup>, and MARCO GRIONI<sup>1</sup> — <sup>1</sup>Ecole Polytechnique Federale de Lausanne, Switzerland — <sup>2</sup>University of Chiba, Japan — <sup>3</sup>University of Tokyo, Japan — <sup>4</sup>Spring-8, Japan

Anatase TiO<sub>2</sub> has been proposed for many applications from transparent conducting panels to photovoltaic- and photocatalytic- devices, as well as memristors. However, little is known about the dynamics of the doped-in charge carriers in this textbook insulator. Recently, we have shown by angle resolved photoemission (ARPES) that these populate the bottom of the conduction band and strongly couple to an optical phonon mode, forming so called large polarons (Moser et al., PRL 110, 196403, 2013).

In the present study, we take the point of view of the phonon. By means of bulk-sensitive resonant inelastic X-ray scattering (RIXS) at the Ti L3 edge. We find that the formation of the polaron cloud involves a single 95 meV phonon along the *c*-axis, besides the 108 meV ab-plane mode previously identified by ARPES. The coupling strength to both modes is the same within error bars, and it is unaffected by the carrier density. This establishes RIXS as a directional and bulk-sensitive probe of electron-phonon coupling in solids (Moser et al. PRL 115, 096404, 2015).

KR 4.4 Thu 16:40 H26

**Polycrystalline organic semiconductors studies by X-ray nano diffraction** — •CLEMENS LIEWALD<sup>1,2</sup>, SIMON NOEVER<sup>1,2</sup>, STEFAN FISCHER<sup>1</sup>, JANINA ROEMER<sup>1</sup>, and BERT NICKEL<sup>1,2</sup> — <sup>1</sup>Fakultät für Physik & Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München — <sup>2</sup>Nanosystems Initiative Munich, Schellingstrasse 4, 80799 München

The efficiency and reliability of organic semiconducting devices depends strongly on the knowledge of the nanoscale arrangement in the active organic layers. Here, we report on the possibilities of X-ray nano-diffraction to characterize polycrystalline organic thin films at beamline ID01, ESRF, before and after its upgrade. The beam diameter in our measurements is 110 nm at 8.9 keV and 350 nm at 20 keV. We find a high beam damage at 8.9 keV compared to only little damage at 20 keV. First, we apply the focused X-ray beam to a multilayer device, with different organic and inorganic layers, and demonstrate the possibility to measure buried microstructures in e.g. the active organic layer under and next to gold electrodes. Second, we explore the local distribution of two polymorphs in a single pentacene thin film.

The lateral shape and distribution of these polymorphs can be mapped with infrared (IR) scanning near-field optical microscopy (SNOM) and is compared to the amplitude from the focused X-ray beam at ID01. In future, the combination of X-ray nanodiffraction with e.g. IR-SNOM

as a correlated microscopy will allow to gain various new insights to the influence of the nanoscale crystallinity on the efficiency of organic electronics devices.

## KR 5: Mitgliederversammlung der FG Kristallographie

Time: Thursday 17:20–18:00

Location: H26

**Wahlen!**