KFM 14: TEM-based Nanoanalysis and Microstructure of thin films (joint session KFM/CPP)

Chair: Bernd Rellinghaus (Dresden Center for Nanoanalysis, TU Dresden)

Time: Thursday 14:10–16:20 Location: HSZ 301

KFM 14.1 Thu 14:10 HSZ 301

The effect of dynamical scattering in ferroelectrics on the measurements of internal electric fields by momentum-resolvedSTEM — •Achim Strauch[1,2], Andreas Rosenauer[3], Andrei Sokolov[4], Evgeny Tsymbal[4], and Knut Müller-Caspary[1,2] — [1]Forschungszentrum Jülich — [2]RWTH Aachen University — [3]IFP Universität Bremen — [4]University of Nebraska-Lincoln

Ferroelectric tunnel junctions (FTJs) are one focus of next-generation memories. With these non-volatile memories, the energy consumption can be reduced. Devices with $BaTiO_3$ tunnel junctions cannot be reversibly polarised at ferroelectric thickness below approximately 3 nm [1]. For investigations, a STEM method would be desirable to map the ferroelectric domain structure in ferroelectric nanofilms exploiting the recently accessible four-dimensional data sets from momentum-resolved STEM [2]. In this contribution, we address the impact of systematic errors arising from dynamical scattering, violated inversion symmetry, sample tilt, and redistributions of electrons due to chemical bonding in a simulation study accompanied by experiments on $BaTiO_3$ and $PbZr_xTi_{1-x}O_3$. The effects of dynamical scattering can lead, depending on thickness, to a systematic error [3] in the order of the expected unit-cell averaged electric fields. Finally the influence of surfaces charges will be discussed.

[1] Garcia et al., Nature Comm. 5, 4289 (2014)
[2] K. Müller et al., Nature Commun. 5, 5653 (2014)
[3] K. Müller et al., Phys. Rev. Lett. 122 (2019)

KFM 14.2 Thu 14:30 HSZ 301

A Novel High-Pressure Tin Oxynitride Sn_2N_2O — •Philipp Gollé-Leidreiter[1], Shrikant Bhat[2], Leonore Wiehl[1], Ute Kolb[1], and Ralf Riedel[1] — [1]Technische Universität Darmstadt — [2]Photon Science DESY

The crystal structure of a novel high pressure high temperature tin oxynitride phase (Sn_2N_2O) was solved via Automated electron Diffraction Tomography (ADT) [1]. The new phase was synthesized from a Sn-N-O precursor at 20 GPa and 1200-1500°C. Due to strong overlaps of symmetrically non-equivalent reflections, the unknown structure could not be solved based on X-ray powder diffraction data. Using the ADT method three dimensional electron diffraction data from a single nanocrystal can be collected in a TEM [2]. The crystal is tilted in 1° steps and diffraction patterns are measured sequentially. Thereby, the reconstructed reciprocal space delivers the unit cell as well as the space group. The intensities of the reflections can be extracted and used to solve the crystal structure via approaches like *direct methods*. The new phase crystallizes in space group Pbcn with the unit cell parameters: a=7.8Å, b=5.53Å, c=5.54Å. The crystal structure could be solved and refined applying kinematic and dynamic theory. It is a Rh_2S_3 type structure where the Sn atoms are sixfold coordinated by O and N atoms. The refined structure compares very well with DFT calculations. This shows the value ADT can provide for the structure solution of high pressure and high temperature materials.

[1]Bhat S, et al. (2019) Chem. Eur. J. 10.1002/chem.201904529
[2]Kolb U, et al. (2019) doi.org/10.1107/S2053520619006711

KFM 14.3 Thu 14:50 HSZ 301

The role of spatial coherence for the creation of and imaging with atom size electron vortex beams — •Darius Pohl[1,2], Stefan Löffler[4], Sebastian Schneider[2,3], Peter Tiemeijer[5], Sorin Lazar[5], Kornelius Nielsch[2], and Bernd Rellinghaus[1,2] — [1]Dresden Center for Nanoanalysis, TU Dresden, D-01062 Dresden, Germany. — [2]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany. — [3]Institute for Solid State Physics, TU Dresden, D-01062 Dresden, Germany. — [4]University Service Centre for Transmission Electron Microscopy, TU Wien, 1040 Wien, Austria. — [5]Thermo Fisher Scientific, PO Box 8066, 5600 KA Eindhoven, The Netherlands.

Recently discovered electron vortex beams (EVBs), which carry quantized orbital angular momenta (OAM), are envisioned to be used in combination with measurements of the electron magnetic circular dichroism (EMCD) to determine the magnetic properties of a material in transmission electron microscopes. Since EVBs can be easily focused down to sub-nanometer diameters, this novel technique bears enormous potential for the quantification of spin and orbital magnetic moments with unrivalled lateral resolution. We use specially designed condenser apertures to generate isolated atom size EVBs with user-selectable OAM. Since the "purity" of the beam regarding the chosen OAM depends on the coherence of the electron source, we have used the monochromator in a double aberration corrected FEI Titan[3] 80-300 microscope to control the degree of this coherence. It will be presented, how a likewise improved coherence will affect the quality of the EMCD measurements.

10 min. break

KFM 14.4 Thu 15:20 HSZ 301

Ferroelectric and structural properties of epitaxial NaxBi1-xTiO3 and BaxSr1-xTiO3 based thin films for electrocaloric studies — •Bruno Magalhaes[1,2], Stefan Engelhardt[1,2], Christian Molin[3], Sylvia Gebhardt[3], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]IFW Dresden, Institute for Metallic Materials, Dresden, Germany — [2]Institute of Material Science, TU Dresden, Dresden, Germany — [3]Fraunhofer IKTS, Fraunhofer Institute for Ceramic Technologies and Systems, Winterbergstraße 28, D-01277 Dresden, Germany

The purpose of our study is to investigate the electrocaloric effect in lead-free epitaxial NaxBi1-xTiO3 (NBT) and BaxSr1-xTiO3 (BST) based thin films. We are focusing on microstructural changes to identify the basic mechanisms of the caloric effects, which might enable a further optimization. Our aim is to investigate the influence of the deposition parameters as well as the functional properties in these material systems. Therefore, NBT and BST based thin films were grown on different single crystalline substrates by pulsed laser deposition. The structural characterization verifies an epitaxial growth of both materials with an additional tetragonal distortion. Temperature and frequency dependent measurements of the dielectric properties as well as polarization were used to determine the temperature of maximum permittivity and the ferroelectric properties, respectively. Finally, we will discuss the impact of the deposition parameters on the structural and functional properties of the grown films. This work is supported by the DFG priority program 1599 Ferroic cooling.

KFM 14.5 Thu 15:40 HSZ 301

Uncloaking structural information of ultra-thin oxide films by surface enhanced Raman spectroscopy — •Mads C. Weber[1], Sebastian Heeg[2], Roman Wyss[3], Martin Sarott[1], Morgan Trassin[1], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Department of Information Technology and Electrical Engineering, ETH Zurich — [3]Department of Mechanical and Process Engineering, ETH Zurich

Strained oxide thin films are a source for properties nonexistent in bulk form such as ferrelectricity in $SrTiO_3$ or altered conductivity in nickelates. These physical properties result commonly from subtle structural distortions. Unfortunately, subtle distortions and specifically oxygen displacements are chronically difficult to probe hindering an in-depth understanding of the phenomena. Here, we introduce surface enhanced Raman spectroscopy (SERS) – a technique so far restricted to molecules and carbon-nanostructures – to scrutinize the structure of oxide thin films. A porous gold membrane deposited on the sample acts as antenna and amplifies the Raman signal of the outer layers only. Using this method, we set the Raman spectra of our model thin film $LaNiO_3$ apart from the substrate giving the important structural insight. Beside information on the strain state of $LaNiO_3$, we identify an ultra-thin surface layer structurally different from the rest of the film. Such a surface layer was so far only theoretically predicted, however, never observed. In general, we anticipate that the introduction of SERS to reign of complex oxides films will help to understand the link between novel physical phenomena and structural distortions.

KFM 14.6 Thu 16:00 HSZ 301

Characterizing self-assembled nanostructures in a hierarchical-structured film by coherent two-dimensional microscopy — •Donghai Li[1], Evgenii Titov[1], Maximilian

Roedel[2], Verena Kolb[2], Sebastian Goetz[1], Roland Mitric[1], Jens Pflaum[2,3], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Lehrstuhl für Experimentelle Physik VI, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), Magdalene-Schoch-Str. 3, 97074 Würzburg, Germany

Self-assembled nanostructures facilitate the development of functional materials with widely tunable properties. Hierarchical architectures consist of nanoscale building blocks spatially modulated by microscale patterns. Despite its relevance for applications and devices, characterization is demanding with existing methods because typically the local molecular-scale assembly pattern within the nanostructure cannot be resolved. Here, we determine nanostructure morphology in a hierarchically structured organic film using coherent two-dimensional (2D) micro-spectroscopy in combination with theoretical modelling of excitonic spectra. We obtain local 2D spectra with diffraction-limited spatial resolution of 260 nm. Using first principles calculations of exciton spectra for model aggregates we connect the experimentally observed signal to the characteristic lengthscale of the nanocrystallites. Thus we obtain a spatial map of nanoscale self-assembly size and confirm it to be correlated with the local slope of the microstructured film surface.