KFM 17: Microstructure, Real Structure and Crystal Defects

Time: Friday 9:30–12:30 Location: TOE 317

KFM 17.1 Fri 9:30 TOE 317

Emitter-Site Specificity of Hard X-ray Photoelectron Kikuchi-Diffraction — •Olena Fedchenko[1], Aimo Winkelmann[2], Sergey Chernov[1], Katerina Medjanik[1], Sergey Babenkov[1], Steinn Agustsson[1], Dmitry Vasilyev[1], Moritz Hoesch[3], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]JGU, Institut für Physik, Mainz, Germany — [2]ACMiN, AGH University of Science and Technology, Krakow, Poland — [3]DESY Photon Science, Hamburg, Germany

High-resolution full-field imaging of (k_x, k_y) photoelectron distributions (angular resolution 0.03°) in a large field of view (up to 20 $Å^{-1}$ dia.) gives access to subtle details in Kikuchi-type diffractograms [1]. This method opens a new avenue to structural analysis via hard X-ray Photoelectron Diffraction (hXPD). We present a theoretical study of the emitter-site specificity by simulating hXPD patterns for arbitrary positions of emitter atoms in the unit cell. Using the Bloch wave approach to photoelectron diffraction from lattice planes [2], the diffraction patterns from an arbitrary number of positions in the unit cell can be obtained simultaneously making use of the reciprocity theorem. Simulations for emitter atoms at various positions in the unit cell of silicon reveal surprisingly strong changes (despite the fact that the entire lattice is kept fixed). The results are compared with measurements for Si doped with Te using ion-implantation [3].

[1] O. Fedchenko et al., New J. of Phys, 21,113031 (2019); [2] A. Winkelmann et al., New J. of Phys. 10, 113002 (2008); [3] M. Hoesch et al., this conference.

KFM 17.2 Fri 9:50 TOE 317

The influence of trace element additions to Al-1.7 at.% Cu alloys: preservation of quenched-in vacancies and atomistic mechanisms supporting θ' — •Torsten E.M. Staab[1], Frank Lotter[1], Uwe Mühle[2], Mohamed Elsayed[3], Danny Petschke[1], Thomas Schubert[4], Alaa M. Ibrahim[3], Reinhard Krause-Rehberg[3], and Bernd Kieback[2,4] — [1]University Wuerzburg, Dep. of Chemistry, LCTM, Roentgenring 11, D-97070 Wuerzburg, Germany — [2]TU Dresden, Institute of Materials Science; Helmholtzstr. 7, D-01069 Dresden, Germany — [3]Martin-Luther-University Halle-Wittenberg; Faculty of Natural Science II; von-Danckelmann-Platz 3; D-06120 Halle, Germany — [4]Fraunhofer IFAM, Winterbergstrasse 28, D-01277 Dresden, Germany

Aluminium-copper alloys receive their strength during hardening by the formation of copper-rich precipitates. Their size, distribution and crystal structure are responsible for their mechanical properties. Adding small amounts of cadmium, indium or tin influences the precipitation behavior as well as the final strength of Al-Cu alloys. Quenched-in vacancies are bound to trace element atoms in the aluminium matrix. Thus, the diffusion behavior of the copper atoms is influenced. For high-purity ternary alloys we investigate the interaction of copper atoms and trace elements (In, Sn, and Pb) with quenched-in vacancies. Annealing the quenched alloys at elevated temperatures leads to finely distributed θ'- precipitates on the nanoscale.

KFM 17.3 Fri 10:10 TOE 317

Using atomic force microscopy to tune functionality at the nanoscale — •Donald M. Evans[1], Theodor S. Holstad[1], Aleksander B. Mosberg[1], Didrik R. Småbråten[1], Per E. Vullum[2], Anup L. Dadlani[1], Zewu Yan[3,4], Edith Bourret-Courchesne[4], Jan Torgersen[1], Antonius T. J. van Helvoort[1], Sverre M. Selbach[1], and Dennis Meier[1] — [1]NTNU, Trondheim, Norway — [2]SINTEF Industry, Trondheim, Norway — [3]ETH Zurich, Zürich, Switzerland — [4]Lawrence Berkeley National Laboratory, Berkeley, USA

The control of conductivity is critical to any electronic device. In this context, oxide materials are particularly interesting as their conductivity can be continuously tuned via an electric field. In addition, they have a plethora of inherent functionalities arising from the electronic degrees of freedom, such as, superconductivity, magnetism, and ferroelectricity. However, utilizing both these changes in conductivity and electronic degrees of freedom simultaneously requires the ability to change one without affecting the other. Usually this is a problem, as the net redox reaction that gives the change in conductivity also affects the electronic degrees of freedom. In this talk, I demonstrate how stable, nanoscale, enhancement of conductivity can be achieved in ferroelectrics without net mass transfer, net change in stoichiometry, or the build-up of spurious electric and chemical gradients. This approach permits both the multiple orders of magnitude change in conductivity and the inherent functionality of oxides to be utilized independently and in parallel to each other.

KFM 17.4 Fri 10:30 TOE 317

Exploring electronic properties of topological insulators using nuclear magnetic resonance — •Robin Guehne and Jürgen Haase — Felix Bloch Institute, Leipzig University, Leipzig, Germany

The investigations of 3-dimensional topological insulators such as Bi_2Se_3 focus chiefly on the gapless surface states that emerge as a consequence of the special energy band inversion near the Fermi level induced by spin-orbit coupling. Not as much studied are the real-space properties of the bulk, although, the band inversion, for example, changes the wave function of the free carriers in the bulk, compared to the topologically trivial counterpart without band inversion.

Recently we have shown that nuclear magnetic resonance (NMR) as a local, bulk probe can detect this band inversion through the electric quadrupole interaction that, in addition, measures the concentration of free carriers, e.g. originating from self-doping effects [1]. Furthermore, our orientation dependent ^{209}Bi NMR experiments in single crystalline Bi_2Se_3 reveal a so far unknown effect in condensed matter – a magnetic field induced charge symmetry that leaves the electric field gradient at the Bi site to rotate rather freely with the external magnetic field B_0 due to spin-orbit coupling as experienced by conduction electrons.

NMR data in external fields up to 17 T, i.e., shifts, linewidths and quadrupole splittings, in three-dimensional topological insulators will be discussed.

[1] R. Guehne, V. Chlan, G. V.M. Williams, S. V. Chong, K. Kadowaki, A. Pöppl, and J. Haase. J. Magn. Res. 302, 34 - 42 (2019)

20 min. break

KFM 17.5 Fri 11:10 TOE 317

Hidden Diversity of Vacancy Orderings in Prussian Blue Analogues — •Arkadiy Simonov[1,2], Hanna B. Boström[2], and Andrew L. Goodwin[2] — [1]Multifunctional Ferroic Materials, Materials Department, ETH Zürich — [2]Inorganic chemistry laboratory, University of Oxford

Prussian blue analogues (PBAs) are a broad and important family of microporous inorganic solids, famous for their gas storage, metal-ion immobilisation, proton conduction, and stimuli-dependent magnetic, electronic and optical properties, The family also includes widely investigated hexacyanoferrate/hexacyanomanganate (HCF/HCM) battery materials. Central to the various physical properties of PBAs is the ability to transport mass reversibly, a process made possible by structural vacancies. In the absence of a better model the distribution of such vacancies was assumed random.

In this talk I would like to present the latest results of analysis of the diffuse scattering from PBA single crystals which show that vacancy show surprisingly strong local ordering. Moreover, the distribution of these vacancies is influenced by crystallisation conditions. Our results establish a clear foundation for correlated defect engineering in PBAs as a means of controlling storage capacity, anisotropy, and transport efficiency.

KFM 17.6 Fri 11:30 TOE 317

Structural defects in silicon observed in situ by X-ray diffraction imaging during heating and solidification — •Maike Becker, Gabrielle Regula, Serge W. Neves Dias, Hadjer Ouaddah, Guillaume Reinhart, and Nathalie Mangelinck-Noël — Marseille Univ, Université de Toulon, CNRS, IM2NP, Marseille, France

Dislocations affect decisively the crystal quality and thus, the minority carrier lifetime, which is problematic for the efficiency of silicon in photovoltaic applications. The understanding of the formation of the dislocation arrangement is of particular importance whenever seeds are part of the Si ingot manufacturing process. To explore the role of seed crystals, this work focuses on dislocation nucleation and mobility in a seed during heating up to the melting point and during the start of

solidification. Synchrotron in situ X-ray diffraction imaging (topography) is used to observe extended crystallographic defects in a silicon wafer. During heating, dislocations are generated at the sample edges and propagate in the sample. We measure their motion which intensifies with increasing temperature and observe their interactions. When solidification is triggered, some dislocations initially present in the seed propagate in the regrown crystal with the solid-liquid interface. The density of these growth dislocations decreases in the up-grown crystal when interacting with $\Sigma 3$ grain boundaries. Besides, the formation of new dislocation sources can be observed during the experiment nearby higher-order grain boundaries.

KFM 17.7 Fri 11:50 TOE 317

Examination of defects and lattice vibrations in rare and common polytypes of Silicon Carbide — •Maximilian von Roeder, Jurek Lange, Detlev Hofmann, Sangam Chatterjee, and Peter Klar — I. Physikalisches Institut and Zentrum für Materialforschung, Justus-Liebig-Universität, 35392 Gießen, Deutschland

Silicon Carbide is a wide band gap semiconductor existing in multiple polytypes. The most common polytypes are 4H- and 6H-SiC, rare ones are 8H- and 21R-SiC. The polytypism has significant effects on various properties of the material, especially the electronic band gap and thermal stability. The polytypism originates from different stacking of the layers composed of SiC_4-tetrahedra. This results in quasi-cubic and quasi-hexagonal lattice sites in the crystal of a polytype. We used Raman-spectroscopy to show the dependence of the A_1 acoustic phonon branch on the stacking type. It can be used as a fast and non-destructive way to classify the polytype at room temperature. Point defects (vacancies and impurities) were studied by electron paramagnetic resonance (EPR) spectroscopy. Furthermore, lattice vacancies are created by high-energy ($E_P = 190$ MeV) proton radiation vacancies in 4H-SiC-samples with fluxes of 10^{11} cm^{-2}, 10^{13} cm^{-2} and 10^{14} cm^{-2}. The EPR-spectra were analyzed in terms of the g-tensor, the exchange splitting (D), and the hyperfine interactions. The results of our investigation will be used to discuss the effects on the electrical properties of the silicon carbide polytypes.

KFM 17.8 Fri 12:10 TOE 317

Investigation of the real structure by means of unconventional methods of the analytical electron microscopy — •Enrico Langer — Technische Universität Dresden, Institut für Halbleiter- und Mikrosysteme, 01062 Dresden, Germany

The primary beam of a scanning electron microscope generates a local X-ray source in the investigated sample, which besides the standard application for the energy dispersive X-ray spectroscopy leads in crystalline volumes directly to lattice source X-ray interferences (Kossel technique). A further possibility consists in a focus of electrons on thin metallic foils (e.g. Fe, Ti) close to the sample surface, which is suited for the generation of a X-ray source in transmission, whereby a tube shields from the bremsstrahlung. Pseudo-Kossel interferences emerge from the diffraction of these divergent X-rays at mono- and polycrystalline material. Beside the X-ray topography this is another method for the mapping and characterization of crystal defects. However, the influence of crystal lattice defects on pseudo-Kossel X-ray interferences was only partly investigated. This work should contribute to a better understanding. The basic investigations range from the real structure characterization of intermetallic alloys to semiconductor materials, such as silicon and GaAs. The deviations from the ideal pseudo-Kossel reflection show the fault of the crystal lattice. These will be assigned to a local section of the original curve on the crystal surface by simulation of complex curves of the 4^{th} order using the further developed program KOPSKO[1]. Especially reflections ruptures can be assigned to the mosaic structure and sub-grains resp., small angle tilt or twist grain boundaries and can be measured with high accuracy. Curve sections with reflection broadening correspond to a local increase of the dislocation density, which were for example found near to grain boundaries in a Fe-Al alloy. Smallest local variations of the lattice constants lead to changes in the position perpendicular to the pseudo-Kossel curve. Even at single-crystals much more complicated regular line structures can be observed, but the formation of models is still not finished.

[1] E. Langer, R. Kurt, S. Däbritz, Cryst. Res. Technol. 34 (1999) 801.