KR 6: Poster: Crystallography in Materials Science

Time: Wednesday 15:00–17:30 Location: P1

KR 6.1 Wed 15:00 P1

Investigation of the Mosaicity of Real Crystals — •Anne Kathrin Hüsecken, Oleg Schmidt, and Ullrich Pietsch — Fakultät Physik, Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen (Germany)

Extinction is the weakening of the diffracted X-ray intensity due to multiple scattering in the crystal. Perfect crystals scatter according to the dynamical theory, but no real crystal is perfect. Ideal imperfect crystals scatter according to the kinematical theory. In most cases, the measured intensities of real crystals are in between both cases and an extinction correction is needed to fulfil the kinematic approach. Most experimentalists use extinction as black box. Present theories dealing with extinction correction start with a finite perfect crystal, then go to an ideal mosaic crystal and at last generalize the theory to a real crystal. These approaches are based on a lot of approximations which are not verified by the experiment. Our approach is to verify the validity of one of the other present extinction theories by independent diffraction experiments with high resolution. The probe system used in the measurements was $Li_2SO_4 \cdot H_2O$. The shape of each Bragg reflection was measured by ω- and ω-2θ-scans. From the FWHMs of these scans of X-ray reflections measured very precisely one can determine the size and the misorientation of the mosaic blocks and also the lattice strain. With these parameters one can experimentally derive the validity of approaches made by certain extinction theories.

KR 6.2 Wed 15:00 P1

Modeling of Defects in Silicon Nitride — •Torsten Weissbach, Steve Schmerler, and Jens Kortus — Institut für Theoretische Physik, TU Bergakademie Freiberg, 09596 Freiberg

Si_3N_4 and Oxynitrides play an important role in todays flash memory technology because of their ability to trap charge and retain it for long time. The long-time trapping occurs in deep centers, electronic states within the large bandgap of the basic materials, which are caused by local impurities and defects. In memory chips, these materials are contained in very thin layers which are assumed to be amorphous. DFT methods are frequently applied to model defects within these materials, but have to be carried out on periodic structure models. One approach is to create large supercells with a nearly amorphous arrangement of atoms. In this case, the crystal structure is strongly disturbed, and local defects are not evident. In another method, defects are modeled by manipulating single atoms in a large supercell of bulk-structure material. Here, we show complex defect models obtained by relocation of several atoms in bulk Si_3N_4, and compare their properties to simpler models as a N vacancy or an O substitutional.

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KR 6.3 Wed 15:00 P1

Polarization dependent Diffraction Anomalous Fine Structure studies of TiO_2. — •Carsten Richter[1,2], Matthias Zschornak[1], Dmitri Novikov[2], Hartmut Stöcker[1], and Dirk C. Meyer[1] — [1]Institute of Experimental Physics, TU Bergakademie Freiberg, Germany — [2]Hamburger Synchrotronstrahlungslabor HASYLAB at DESY, Germany

Diffraction Anomalous Fine Structure (DAFS) is, like X-Ray Absorption Fine Structure (XAFS), a method suitable to study the local electronic structure of a certain type of atoms in the crystal. In contrast to absorption spectroscopy atoms of the same type but different crystallographic sites can be distinguished, due to the combination of spectroscopy and diffraction. Near an absorption edge, the atomic scattering factor becomes dependent of the polarization and direction of the incident and the reflected beam. Reflection conditions based on the crystal's symmetry can be used to eliminate polarization or direction independent parts. This and the variation of the polarization with respect to the crystal allows a closer insight into the types of electronic transitions involved in the scattering process.

Here we present a detailed DAFS study of rutile single crystals with different densities of oxygen vacancies including measurements and modeling of the energy and polarization dependence of the scattered intensity. Recent results of its separation into the 2 polarization states using a polarization analyzer are included. The measurements have been carried out for rutile reflections 001 and 111 at beam lines C, E2 and W1 of the HASYLAB at DESY.

KR 6.4 Wed 15:00 P1

X-ray diffractometry of magnetic (Ga,Mn)As epitaxial layers — •Vaclav Holy[1], Xavier Marti[1], Lukas Horak[1], Vit Novak[2], and Tobias Schuelli[3] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague, Ke Karlovu 5, 121 16 Prague, Czech Republic — [2]Insititute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 00 Prague, Czech Republic — [3]ESRF, BP220, 38043 Grenoble, France

The magnetic Mn ions in (Ga,Mn)As epitaxial layers can be found in substitutional and two types of interstitial positions, however only the magnetic moments of the substitutional Mn ions can be ferromagnetically ordered, and the Mn interstitials are detrimental for the ordering. The determination of the density of Mn ions in different lattice positions is therefore an important task. We have determined the densities of Mn substitutional and interstitial ions in (Ga,Mn)As by high-resolution x-ray diffractometry both using a single wavelength, and by measuring the dependence of the diffracted intensity on the photon energy around the MnK absorption edge (anomalous diffraction). In the former method, the dependence of the lattice parameter of the (Ga,Mn)As alloy on the Mn densities must be known a-priori. The latter approach does not use the value of the lattice parameter, however it can be realized only by means of synchrotron radiation. We have used both methods for the study of the kinetics of out-diffusion of Mn interstitials from (Ga,Mn)As layers during post-growth annealing.

KR 6.5 Wed 15:00 P1

Oxygen nonstoichiometry of tetragonal La2-xSrxCuO4-δ (x = 0.15 - 1.2) and in situ XPS studies at elevated temperatures — •Daria Mikhailova[1], Vladimir Alyoshin[2], Steffen Oswald[1], and Helmut Ehrenberg[1] — [1]IFW Dresden, Helmholtzstr. 20 01069 Dresden, Deutschland — [2]Moskauer Staatliche Lomonossov Universität, Vorobyovy Gory, 119992, Moscow, Russia

The peculiarities of oxygen nonstoichiometry (δ) in tetragonal La2-xSrxCuO4-δ solid solution with x(Sr) = 0.15 - 1.2 were studied by XRD, NPD, in situ high-temperature XPS and chemical analysis. Temperature dependences of oxygen nonstoichiometry, $\delta = \delta(T)$, were obtained for different Sr-contents at 1 bar O2. Two types of charge compensation during replacement of lanthanum by strontium are discussed: an increase of the average copper oxidation state or a formation of oxygen vacancies. The average copper oxidation state V(Cu) exhibits a maximum of 2.32 at x(Sr)=0.6, while δ increases with x(Sr). Oxygen vacancies are unambiguously located on the 4c site ({CuO2}-plane) for compositions with different strontium contents, which electronic state is described by the O2p core electron peak at about 531 eV. Thermal stability of the solid solution in vacuum is associated with the extraction of practically the entire oxygen from CuO2-layers and the formation of Cu+ at least in the surface-near region. The higher average copper oxidation state after synthesis in the Sr-rich phases in comparison with the Sr-poor compositions prevents oxygen removal and the formation of Cu+ and, therefore, stabilizes the structure during heating in vacuum.