KR 7: Crystallography in Materials Science (jointly with DF)

Time: Thursday 14:00–16:45 Location: HSZ 101

Invited Talk KR 7.1 Thu 14:00 HSZ 101

Crystallography of Nanowires — •Julian Stangl[1], Dominik Kriegner[1], Christian Panse[2], Bernhard Mandl[1,3], Kimberley A Dick[3], Mario Keplinger[1], Johan M Persson[4], Philippe Caroff[3,5], Daniele Ercolani[6], Lucia Sorba[6], Friedhelm Bechstedt[2], and Günther Bauer[1] — [1]Johannes Kepler University Linz, Austria — [2]Friedrich-Schiller-Universität Jena, Germany — [3]Lund University, Sweden — [4]Technical University of Denmark — [5]IEMN, UMR CNRS, France — [6]Scuola Normale Superiore Pisa, Italy

Semiconductor nanowires are interesting not only from physical and technological viewpoints, but also in a crystallographic sense. While most III-V semiconductors, except nitrides, crystallize exclusively in the cubic zinc-blende lattice in bulk or epitaxial layers, in nanowires very often hexagonal modifications such as wurtzite, but also the more complex 4H structure are observed. The wires grow mainly along the cubic <111> directions, where those lattice structures on first sight differ only by the stacking sequence of bilayers, changing from fcc to hcp. Detailed x-ray diffraction investigations for InAs and InSb nanowires reveal, however, that beside the stacking sequence also the atomic distances change, so that the unit cells deform compared what would be expected from a simple change of stacking. Comparisons to density functional theory calculations are in excellent agreement with the experimental data, and the combination of x-ray diffraction and theoretical calculations allow explaining the reason for the observed changes in atomic distances.

KR 7.2 Thu 14:45 HSZ 101

The Crystal structure of InAs nanorods grown onto Si[111] substrate — •Anton Davydok[1], Andreas Biermanns[1], Steffen Breuer[2], Manos Dimakis[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Festkörperphysik, Universität Siegen, Walter-Flex-Str. 3,57072, Siegen, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7,10117 Berlin, Germany

Nanowires are of particular interest due to the ability to synthesize heterostructures in the nanometer range. It was found that nearly any AIIIBV semiconductor material can be grown as NWs onto another AIIIBV or group IV [111] substrate independent from lattice mismatch. We presented an X-ray characterization of InAs NRs on Si [111] grown by assist free MBE method. Lattice mismatch of this materials is 11%. For study of strain realizing we concentrated our research on initial stages of growth process investigating samples set with different growth time. Using synchrotron radiation we have performed experiments in symmetrical and asymmetrical out-of plane scattering geometry and grazing-incidence diffraction. Combining the results we were able to characterize the transition between silicon silicon substrate and InAs NWs. We find in-plane lattice mismatch of -0.18% close to the interface compared to InAs bulk material. With help of microfocus setup we are able measure structural paramters of single NWs to determine the strain accomodation as function of NW size. In particular using asymmetric wurzite-sensitive reflections under coherent beam illumination we could quantify the number of stacking faults. In the talk we present details of the analysis and first simulation results.

KR 7.3 Thu 15:00 HSZ 101

X-ray characterization of Au-free grown GaAs nanowires on Si — •Andreas Biermanns[1], Steffen Breuer[2], Anton Davydok[1], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Semiconductor nanowires (NW) are of particular interest due to the ability to synthesize single-crystalline 1D epitaxial structures and heterostructures in the nanometer range. However, many details of the growth mechanism are not well understood. In this contribution we present a x-ray diffraction study of the early stage of Au-free GaAs nanowire growth on Si(111)-substrates with native oxide using the nano-focus setup available at the ID1 beamline of ESRF. The GaAs NWs were grown by molecular beam epitaxy (MBE), and their formation was induced by Ga droplets. Using a nanometer-sized x-ray beam, size and lattice parameters of individual wires were measured separately. Using asymmetric x-ray diffraction on particular zinc-blende (ZB) and wurtzite (W) sensitive reflections, we show that under the used conditions the NW growth starts with predominantly WZ phases and continues mainly in ZB phase. In addition we can show that the WZ segments of the NWs exhibit a different vertical lattice parameter compared to the zinc-blende segments. A combination of x-ray diffraction from single wires and grazing incidence diffraction shows that the base of the NW is compressively strained along the inplane direction. This strain is released within 20nm from the substrate-interface.

15 min. break

Invited Talk KR 7.4 Thu 15:30 HSZ 101

New Grounds in Materials Science: Complex Metallic Alloys — •Michael Feuerbacher — Institut fuer Festkoerperforschung, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany.

Complex metallic alloys (CMAs) represent a class of materials increasingly receiving scientific attention. These materials possess characteristic structural features substantially deviating from those of simple metals. They have large lattice constants and, correspondingly, a high number of atoms per unit cell, ranging from some ten to some thousands. Their local order is dominated by icosahedral-symmetric atom coordination in the form of concentric cluster shells. These characteristic structural features are at the origin of novel physical properties.

Due to the crucial structure-property relations, transmission electron microscopy is an inevitable tool for the understanding of the physical properties of CMAs. We will present structural characterizations of various CMA materials by state-of-the-art techniques, such as aberration-corrected transmission electron microscopy and high-angle annular dark field scanning transmission electron microscopy. We will review recent experimental investigations of the physical properties of CMAs, and discuss these in the light of the particular cluster substructure. Basic scientific phenomena will be addressed, such as novel structural defects and deformation mechanisms, as well as application related issues, for example the use of CMAs as catalysts, as thermoelectric materials, and for digital data storage.

KR 7.5 Thu 16:15 HSZ 101

Local electronic structure of Ruddlesden-Popper films - a combined DFT and ELNES study — Thomas Riedl[1,2], Thomas Gemming[2], Torsten Weissbach[3,4], Gotthard Seifert[4], Emanuel Gutmann[5], Matthias Zschornak[6,7], Dirk C. Meyer[5,6], and •Sibylle Gemming[7] — [1]Werkstoffwissenschaft, TU Dresden, D-01062 Dresden — [2]IFW Dresden, PF 270116, D-01171 Dresden — [3]Theo. Physik, TU-BA Freiberg, D-09596 Freiberg — [4]Phys. Chemie, TU Dresden, D-01062 Dresden — [5]Strukturphysik, TU Dresden, D-01062 Dresden — [6]Exp. Physik, TU BA Freiberg, D-09596 Freiberg — [7]HZ Dresden-Rossendorf, PF 510119, D-01314 Dresden

Ternary oxides with the composition $AO(ABO_3)_n$, the Ruddlesden-Popper (RP) phases, and derived quaternary phases are versatile materials with complex structure-property relationships; due to their unusual conductivity properties such RP phases have attracted recent interest as materials for solid-oxide fuel cells or as thermoelectric. The present study focuses on the parent phases with A = Sr and B = Ti. Electron energy-loss near-edge fine structures of the $SrO(SrTiO_3)_{n=1}$ Ruddlesden-Popper system and of the reference compounds $SrTiO_3$ and SrO are analyzed by comparison with calculations. The fine structures of sol-gel-grown RP films have been experimentally recorded. All-electron density-functional calculations indicate that the appearance and shape of the experimental O-K and Ti-$L_{2,3}$ fine structure features result from the crystallography-dependent electronic structure of the investigated oxides, which - already without further modification - display technologically interesting dielectric and lattice properties.

KR 7.6 Thu 16:30 HSZ 101

Modeling the environment-controlled morphology changes of adsorbed two-component nanoparticles — •Sibylle Gemming[1], Gintautas Abrasonis[1], and Matthias Krause[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, PF 510119, D-01314 Dresden, Germany. — [2]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany.

The morphology and the local composition of binary nano-particles from two immiscible components are driven by the local interactions at the different interfaces within the material system. Especially in

small nano-particles, atoms at interfaces cover a large part of the total amount of atoms. Therefore, the interface energetics crucially influences the relative stabilities of different possible atom arrangements both at the surface of the particles and at the interface with the support. Such a complex system can be mapped to a two-component phase-field model with a set of complex boundary conditions at the interfaces of the particle with the support and with the surrounding atmosphere. Numerical simulations have been performed to describe the morphology evolution of such particles in dependence on the external physical conditions. The results rationalize recent observations on the structural changes of oxide-supported bimetallic nano-particles cycled in oxidizing and reducing atmospheres. Funding via the ECEMP project D1 (EU-EFRE) is gratefully acknowledged.