KR 10: Crystallography in Nanoscience

Time: Thursday 9:30–12:00 Location: E 124

Invited Talk KR 10.1 Thu 9:30 E 124

On polytypism in III-V nanowires — •Friedhelm Bechstedt[1], Abderrezak Belabbes[1], Christian Panse[1], Jürgen Furthmüller[1], Dominik Kriegner[2], and Julian Stangl[2] — [1]Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria

Nanowires (NWs) based on III-V semiconductors, whose bulk crystals crystallize in zinc-blende structure, are usually grown in [111]B direction. Therefore, their bond stacking fluctuates, and the formation of different polytypes is a common phenomenon in NWs. The properties of the hexagonal 6H, 4H, and 2H polytypes are however modified with respect to the cubic zinc-blende (3C) structure.

A systematic study of structural and electronic properties of the Ga-V and In-V compounds (V = P, As, Sb) is reported for four polytypes. The lattice-constant and internal-cell parameters are derived within well-converged density-functional calculations within the local density approximation (LDA) and discussed versus the polytype hexagonality. The comparison with recent X-ray diffraction measurements shows excellent agreement and clear trends.

The quasiparticle electronic structures are computed with high accuracy including spin-orbit interaction applying a recent calculation scheme, the LDA-1/2 method. The fundamental gaps increase with the hexagonality. The results are used to derive band offsets between different polytypes. We predict a type-II heterocrystalline character for the junctions between two polytypes in agreement with spectroscopic studies.

KR 10.2 Thu 10:00 E 124

Crystal structure of InAs on Si(111) substrate — •Anton Davydok[1], Emmanouil Dimakis[2], Andreas Biermanns[1], 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

We present results of X-ray diffraction analysis of InAs nanowire (NW) grown by catalyze-free molecular beam epitaxy on silicon (111) substrate. Independent from lattice mismatch of 11% the NWs grow with their bulk lattice parameter directly on bare silicon with absence of buffer layer or silicon native oxide layer. The structure of individual NWs has been characterized using a beam nano-focus beam spot of few 100nm*. Using coherent beam illumination certain Bragg peaks if individual NWs display speckle-like diffraction pattern due to particular sets of stacking faults separating wurzite and zinc-blende like structural units. Arrangement and density of stacking faults in particular NWs was estimated via modelling. In addition we characterized parasitic InAs islands appearing in addition to NWs which appear entirly in zinc-blende structure.

KR 10.3 Thu 10:20 E 124

In-situ 3D reciprocal space mapping during mechanical deformation — •Thomas Cornelius[1], Anton Davydok[2], Dina Carbone[3], Vincent Jacques[3], Raphael Grifone[3], Marie-Ingrid Richard[1], Till Hartmut Metzger[4], Tobias Schülli[3], Ullrich Pietsch[2], and Olivier Thomas[1] — [1]IM2NP, CNRS, Marseille, France — [2]Siegen University, Siegen, Germany — [3]ESRF, Grenoble, France — [4]MPI of Colloids and Interfaces, Potsdam, Germany

In recent years, low-dimensional materials attracted enormous attention due to size effects which originate from the spatial confinement of the nanostructures affecting their properties. At the beamline ID01 at ESRF, an in-situ AFM was developed for mechanical studies on nanostructures in combination with nanofocused XRD. The X-ray beam is focused to few hundred nanometers and the diffracted X-rays are recorded by a 2D detector. To record the complete structural change during deformation, it is mandatory to measure in-situ the 3D intensity distribution. Since any movement of diffractometer motors induces vibrations leading to the destruction of the AFM-tip and/or the nano-object during compression, ordinary rocking curves cannot be applied. We developed a novel energy tuning approach which allows for the acquisition of 3D-XRD maps during in-situ compression tests and, thus, giving access to the deformation of the structure under investigation. Here, we will present in situ 3D-XRD studies on SiGe islands which served as a model system.

KR 10.4 Thu 10:40 E 124

Structure - stoichiometry relationship of mixed $Ce_{1-x}Pr_xO_{2-\delta}$ (x = 0-1) oxides on Si(111) — •Marvin Zoellner[1], Marcus Bäumer[2], Michael Reichling[3], Henrik Wilkens[3], Joachim Wollschläger[3], Peter Zaumseil[1], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]Universität Bremen, IAPC, Leobener Str. NW2, 28359 Bremen — [3]Universität Osnabrück, Fachbereich Physik, Barbarastr. 7, 49076 Osnabrück, Germany

Cerium and praseodymium oxide thin films are of interest for model catalytic studies. When grown by molecular beam epitaxy on Si(111), CeO_2 exists in the fluorite lattice. Praseodymium prefers the 3+ state as Pr_2O_3, which has either a cubic bixbyite or hexagonal crystal structure. A mixture of both oxides enables to engineer the properties of the catalyst, due to different redox reactivities and lattice alteration. Before model catalytic studies can be carried out, the correlation between crystal structures and stoichiometries of the mixed $Ce_{1-x}Pr_xO_{2-\delta}$ layers must be clarified. We monitored the growth by reflection high energy electron diffraction. X-ray photoemission spectroscopy was applied to determine the stoichiometry. Laboratory and synchrotron based X-ray diffraction was carried out to investigate the crystal structure. The study revealed that $Ce_{1-x}Pr_xO_{2-\delta}$ keeps the Ce^{4+} related fluorite lattice for low praseodymium concentrations (x = 0.30). However, the crystal lattice is dominated by the Pr^{3+} state for medium (x = 0.65) and high (x = 0.75) Pr concentrations so that bixbyite and hexagonal structures are formed, respectively.

KR 10.5 Thu 11:00 E 124

Crystal size and axial stress effects on the B4 to B1 phase transition pressure in AlN and ZnO nanocrystals investigated with second harmonic generation (SHG) — •Leonore Wiehl, Lkhamsuren Bayarjargal, and Björn Winkler — Institut für Geowissenschaften, Goethe-Universität, 60438 Frankfurt/Main, Germany

The transition pressure from the hexagonal (B4) to the cubic (B1) phase is shifted to higher pressures in nanocrystals when compared to bulk crystals for GaN, InN, CdSe or ZnO [1]. Only in AlN a shift to lower pressure was reported [2]. The influence of deviatoric stress was shown to reduce the transition pressure of bulk ZnO from 11 to 9.3 GPa [3]. Here, we present our results on nanocrystals of ZnO and AlN. Pressures up to 30 GPa were generated in diamond anvil cells (DACs), loaded with Ne gas for hydrostatic or KCl for non-hydrostatic conditions. The phase transition was detected by the vanishing of the second harmonic generation signal when going from the acentric (B4) to the centrosymmetric (B1) phase. Our results confirm the shift of transition pressures in nanocrystalline ZnO by 2-3 GPa to higher and in AlN by ∼10 GPa to lower pressures relative to the bulk crystals in accordance with the values reported [1,2] in the hydrostatic case. For the non-hydrostatic loadings transition pressures were reduced by 2-3 GPa. Financial support from the DFG (Ba 4020) is gratefully acknowledged.

[1] J. Z. Jiang et al., Europhys. Lett. 50 (2000) 48-53 [2] Z. Wang et al., J. Phys. Chem. B 108 (2004) 11506-11508 [3] L. Bayarjargal et al., Appl. Phys. Lett. 95 (2009) 061907(3p)

KR 10.6 Thu 11:20 E 124

Manipulation of Ge quantum dot ordering in alumina matrix by deposition conditions — •Maja Buljan[1], Carsten Baehtz[2], Václav Holý[3], Nikola Radić[1], Olga Roshchupkina[2], Slawomir Prucnal[2], Arndt Muecklich[2], Václav Valeš[3], Sigrid Bernstorff[4], and Joerg Grenzer[2] — [1]Ruder Bošković Institute, Croatia — [2]Helmholtz Zentrum Dresden Rossendorf, Gremany — [3]Charles University in Prague, Czech Republic — [4]Sincrotrone Trieste, Italy

We present an investigation of ordering and PL properties of Ge QDs in an alumina matrix formed by magnetron-sputtering deposition of (Ge+Al2O3)/Al2O3 multilayers. The self-assembly process occurs during the deposition and results with the formation of three-dimensional quantum dots lattices. We investigate the dependencies of the size and ordering properties on the deposition temperature, rotation of the substrate holder and direction of the incoming flux of Ge

during the deposition process. The results of the investigation show that tuning the deposition temperature enables manipulation with QD sizes and their mutual distances. We show that the ordering of QDs obtained by deposition on fixed substrate holder leads to the formation of a quantum dot crystal, while the rotation of substrate holder leads to randomly rotated domains with regular ordering. The observed phenomenon is explained by a combination of the surface morphology effect on the nucleation positions of Ge quantum dots with a lateral inhomogeneity of the ad-atom flux. In addition, we show that the resulting quantum-dot lattices have size-dependent PL properties.

KR 10.7 Thu 11:40 E 124

In-situ observation of the Self-assembled growth of ordered Ge nanocrystals embedded within a dielectrical matrix — •Joerg Grenzer[1], Maja Buljan[2], Olga Roshchupkina[1], Carsten Baehtz[1], and Václav Holý[3] — [1]Helmholtz Zentrum Dresden Rossendorf, Gremany — [2]Ruder Bošković Institute, Croatia — [3]Charles University in Prague, Czech Republic

We report on an in-situ X-ray investigation of a self-assembled growth of Ge nanocrystals embedded in a dielectrical matrix forming a *BCC*-like super structure. Such a material could be a key element for the development of a new generation of solar cells extending the spectral range for energy conversion. Using small angle scattering techniques and X-ray diffraction the formation of crystalline Ge nanoparticles during growth and annealing was studied in-situ at the BM20 beam line at that ESRF using a process chamber for magnetron sputter deposition and annealing that can be inserted into the goniometer. A single some 100nm thick Ge+Al_2O_3 layer using magnetron sputtering was deposited at an elevated substrate temperature. The self-assembly during growth or subsequent annealing results in the formation of a well ordered three-dimensional *BCC*-like quantum dot lattice within the whole deposited volume. The formed nanocrystals are very small in size ($< 4.0nm$), with a very narrow size distribution and a large spatial density. The parameters of the formed super structure can be directly influenced by changing the deposition parameters. The self-ordering of the quantum dots is explained by diffusion mediated nucleation and surface morphology effects.