HL 81: Heterostructures and interfaces

Time: Thursday 15:00–18:15 Location: EW 201

HL 81.1 Thu 15:00 EW 201

Structural and Electronic Properties of Si-ZnO and Si-In_2O_3 Interfaces from First Principles — •Benjamin Höffling[1,2] and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]European Theoretical Spectroscopy Facility (ETSF)

We develop a method for the construction of atomic models of heterostructural interfaces based on coincidence lattices, maximum bond saturation, and total energy minimization, which enables us to construct model geometries for the interface between diamond structure Si, *bcc*-In_2O_3 and wurtzite-ZnO. In particular we investigate the Si(001)-In_2O_3(001), the Si(001)-ZnO($10\bar{1}0$) and the Si(001)-ZnO($20\bar{2}3$) interface by means of density functional theory (DFT). We predict electronic properties of the interface using both DFT and modern quasiparticle theory based on semilocal exchange-correlation functionals and examine electronic band discontinuities as well as the details of the interface electronic structure. The influence strain and charge transfer on the electronic density of states is discussed.

The band offsets and, hence, the efficiency of Si-TCO based devices depend crucially on the charge transfer at the interface, i. e. on the nature of the chemical bonds at the junction.

HL 81.2 Thu 15:15 EW 201

Computer Simulation of Growth Kinetics of Compound Semiconductors — •Jan Oliver Oelerich and Sergei D. Baranovskii — Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg

Growth of III/V semiconductor compounds on Si substrates is currently in the focus of experimental and theoretical research because of its promising applications in functionalization of semiconductors. While surface structures and properties of the grown materials are experimentally well accessible, little is known about the formation and structural characteristics of the interfaces between the Si substrate and the III/V semiconductor compound. To gain insight into the intermediate stages of epitaxial growth and the interface properties, we developed a Kinetic Monte Carlo (KMC) computer simulation package for the theoretical study of the kinetic characteristics of epitaxial growth. Two particular problems were addressed in the simulations. First, it was recently observed that growth of GaP on the Si-001 surface leads to significant intermixing of the two materials at their interface. In our simulation we were able to identify the driving forces of the intermixing and accurately reproduce the experimentally observed features. Second, melt-back etching of Ga droplets on the Si-001 surface was simulated. In a recent experimental study it was shown that deposition of Ga onto a Si substrate leads to formation of metallic Ga droplets, etching large, pyramidally shaped structures into the bulk Si. We can reproduce this behaviour in the simulation and thereby study intermediate stages of the etching during the Ga deposition.

HL 81.3 Thu 15:30 EW 201

Band alignment in lateral two-dimensional heterostructures — Stephan Vercauteren, Ortwin Leenaerts, Bob Schoeters, and •Bart Partoens — University of Antwerp, Department of Physics, Belgium

The properties of semiconductor interfaces is mainly determined by the alignment of their respective band structures. Various methodologies have been devised to obtain the band alignment for bulk semiconductors, ranging from the simple alignment of vacuum potentials to the explicit simulation of the heterostructure with first-principles methods. When the dimensionality of the semiconductors is reduced, several problems with these alignment methods arise. Especially in-plane heterostructures, which consist of laterally connected 2D crystals, are more difficult to treat. Naive reasoning suggests that the simple alignment of the vacuum levels above each material is sufficient to determine the band alignment, but this simple reasoning is incorrect. We demonstrate that the vacuum potential is generally different above different 2D materials and that this difference depends crucially on the thickness of the involved materials. Furthermore, care should be taken to obtain the band alignment through heterostructure modeling with first-principles methods. The boundary conditions have a strong impact on the band alignment which needs to be corrected for.

HL 81.4 Thu 15:45 EW 201

Stability and capping of magnetite ultra-thin films — •Karsten Fleischer, Ozhet Mauit, and Igor V. Shvets — School of physics, Trinity College Dublin, Ireland

Ultrathin films of Fe_3O_4 have been grown epitaxially on nearly lattice matched MgO(001). The stability of 4 nm thick films in ambient air and under annealing in an oxygen atmosphere at 570K has been studied. By magneto optical and Raman measurements, we can confirm the presence of the Fe_3O_4 phase and the formation of a maghemite top layer passivating the Fe_3O_4 thin film. In a second step, we are able to demonstrate that this top layer oxidation in ambient air can be prevented by a 2 nm thick magnesium ferrite passivation layer, while a thicker 20 nm MgO layer prevents oxidation even at elevated temperatures.

HL 81.5 Thu 16:00 EW 201

An XPS study on copper oxide based solar cells — •Benedikt Kramm, Philipp Hering, Philipp Schurig, Fabian Michel, Angelika Polity, and Bruno K. Meyer — 1. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

For semiconductor hetero junctions the energy band alignment is one of the crucial factors which deliver a judgment for a successful operating device. We fabricated hetero junctions based on p-type cuprous oxide with n-type $Al_xGa_{1-x}N$ (first type) and $Mg_xZn_{1-x}O$ (second type) as window layer. The $Al_xGa_{1-x}N$ film was grown epitaxial on sapphire substrates whereas the copper oxide was deposited on top by RF-magnetron sputtering. $Mg_xZn_{1-x}O$ was similar deposited on sapphire substrates by RF-magnetron sputtering and again finally Cu_2O was deposited. An advantage of $Mg_xZn_{1-x}O$ compared to $Al_xGa_{1-x}N$ is the low cost fabrication even on a large scale as well as the sustainability of the elements. But it is well known that $Mg_xZn_{1-x}O$ has its limits in conductivity with increasing Mg content. Nevertheless, it might be possible to align the conduction bands of $Mg_xZn_{1-x}O/Cu_2O$ hetero junctions and thus to force up the efficiency in power conversion. Using X-ray photoelectron spectroscopy (XPS), we figured out that the conduction band offsets are getting smaller with increasing Al content for the first type of hetero structures. A similar trend is observable for Mg in the second type. Here, we will present and compare the band offset results. Another focus is on the intermixing at the oxygen-nitrogen and oxygen-oxygen interfaces and how it affects the band alignment.

HL 81.6 Thu 16:15 EW 201

Depth dependence of the ionization energy of shallow hydrogen donor states in ZnO and CdS — •Thomas Prokscha[1], Hubertus Luetkens[1], Elvezio Morenzoni[1], Gerard Nieuwenhuys[1,2], Andreas Suter[1], Max Döbeli[3], Michael Horisberger[4], and Ekaterina Pomjakushina[4] — [1]LMU, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Kamerlingh Onnes Laboratory, Leiden University, 2300 RA Leiden, The Netherlands — [3]Ion Beam Physics, ETH Zurich, CH-8093 Zurich, Switzerland — [4]LDM, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

The ionization energy of shallow hydrogen-like muonium (Mu) donor states in nominally undoped ZnO and CdS (0001) crystals has been measured in a near-surface region (10 - 180 nm depth) by using low-energy muons, and in the bulk using conventional muon spin rotation (μSR) [1]. The implantation depth of the muons is varied by tuning the implantation energy of the low-energy muons between 2.5 and 30 keV. The ionization energy of the shallow Mu donor is lowered by about 10 meV compared to its bulk value at a mean depth of 100 nm, and continuously decreasing on approaching the surface. At a depth of about 10 nm the ionization energy is reduced by 25 - 30 meV. The same reduction is observed at a Au/ZnO interface. We attribute this change to the presence of electric fields due to band bending at the surface/interface. Using a simple one-dimensional model the depth profile of the electric field can be determined.

[1] T. Prokscha et al., arXiv:1408.6972, accepted for publication in Physical Review B.

Coffee break

HL 81.7 Thu 16:45 EW 201

Strain-relaxation in GaAs / InGaAs core-shell nanowire heterostructures grown by MBE onto Si(111) — •Ali Al Hassan[1], Andreas Biermanns[1], Emmanouil Dimakis[2], Ryan B. Lewis[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Naturwissenschaftlich-Technische Fakultät der Universität Siegen, 57068 Siegen, Germany — [2]Paul-Drude- Institute für Festkörperelektronik, Hausvogteiplatz 3, 10117 Berlin, Germany

Core-shell semiconductor nanowires (NW) can be grown onto various substrates without inclusion of misfit dislocations due to the strain release towards the NW side planes. This approach offers the possibility to form radial hetero-structures (HS) between highly lattice-mismatched materials but the process of strain relaxation is not fully understood.

We investigate strain interaction and relaxation in GaAs/InxGa1-xAs/GaAs NWHS grown by MBE onto silicon (111). X-ray diffraction measurements along [111] show, independent from GaAs core and InGaAs shell thickness ratio (x_In= 25% in shell thickness of 17nm), only one out-of plane Bragg peak corresponding to a solid solution with the total In content composed in the NW (Vegards law). On the other hand, X-ray measurements along the (1-10) and (2-1-1) NW side plane show separate peaks for core and shell materials with a mismatch corresponding to an In content in the shell closer to the nominal value but different along the direction normal to NW side planes and normal to NW edges. The data are interpreted in terms of finite element calculations revealing the complexity of strain relaxation mechanism.

HL 81.8 Thu 17:00 EW 201

A molecular statics study of strain fields and defect stability in axial-heteroepitaxial nanopillars — •Thomas Riedl[1,2] and Jörg Lindner[1,2] — [1]University of Paderborn, Department of Physics, Warburger Straße 100, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), Warburger Straße 100, 33098 Paderborn, Germany

Semiconductor nanopillars containing a heteroepitaxial junction in the axial direction are attractive for electronic and optoelectronic applications, owing to the high elastic relaxation of misfit strains and the possibility to modify the electronic band structure by means of strain. Compared to planar substrates axial-heteroepitaxial nanopillars can accomodate larger misfits without formation of misfit-related defects. Previous studies predicting the stability of misfit dislocations in axial-heteroepitaxial nanopillars or nanowires used different variants of analytic continuum theory or the finite element method. In the present contribution we investigate the strain fields and the stability of misfit dislocations in zinc blende InAs/GaAs nanopillars by means of atomistic molecular statics simulation. Because of its applicability to various bonding configurations and availability of suitable parametrizations the Tersoff potential is employed. The stability of the coherent defect-free state and of the dislocated state is analyzed in terms of the pillar dimensions and the dislocation configuration, i.e. dislocation type and position for both [001] and [111] pillar axis directions. The results are compared with the predictions of continuum approaches and with experiments reported in the literature.

HL 81.9 Thu 17:15 EW 201

Time-resolved *in situ* spectroscopy during formation of single-domain GaP/Si(100) heterointerfaces — •Oliver Supplie[1,2], Matthias May[1,2], Andreas Nägelein[1], Gabi Steinbach[3], Oleksandr Romanyuk[4], Frank Grosse[5], Peter Kleinschmidt[1,2], Sebastian Brückner[1,2], and Thomas Hannappel[1,2] — [1]TU Ilmenau, FG Photovoltaik — [2]Helmholtz-Zentrum Berlin, Solar Fuels — [3]Helmholtz-Zentrum Dresden-Rossendorf — [4]Institute of Physics, Academy of Sciences of the Czech Republic — [5]Paul-Drude Institut, Berlin

Though III-V/Si(100) heterointerfaces are essential for future epitaxial high-performance devices, their atomic structure is a historic open question. We study the formation of the GaP/Si(100) heterointerface time-resolved with reflection anisotroppy spectroscopy during pulsed GaP nucleation on almost single-domain Si(100) surfaces [1] in CVD ambient. A terrace-related dielectric anisotropy evolves about 100 meV below the E_1 critical point energy of silicon and agrees well with a GaP/Si(100) interface dielectric anisotropy (IDA) calculated from thicker GaP epilayers on Si(100).[2] X-ray photoelectron spectroscopy reveals a chemically shifted contribution of the P and Si emission lines, which quantitatively correspond to about one monolayer and establish similarly quick as the IDA.[2] We attribute this contribution to Si–P bonds at the heterointerface,[2] which were suggested recently.[3]

[1] Brückner et al., *Phys. Rev. B* **86** : 195310, 2012.
[2] Supplie et al., *J. Phys. Chem. Lett.* submitted, 2014.
[3] Supplie et al., *Phys. Rev. B* **90** : 235301, 2014.

HL 81.10 Thu 17:30 EW 201

Structural investigations of graded buffer systems in the TEM — •Florian Aumeier, Josef Loher, Christian Neumann, Dominique Bougeard, Daniel Henzler, Johannes Wild, Felix Schwarzhuber, and Josef Zweck — Institute of Experimental and Applied Physics, Regensburg, Germany

We investigated quantum well (QW) structures in epitaxially grown GaAs and SiGe graded buffer systems with [001] as growth direction. In these systems the strain induced by the lattice constant mismatch is relaxed by intentional defects in a metamorphic buffer system. The aim was to analyze the crystal quality of the system, in particular the defect free growth of the QW itself. Our focus lies on the detection and characterization of crystal defects with transmission electron microscopy (TEM). Besides the normal Bright Field investigations we used the weak beam dark field (WBDF) method to characterize the different perfect and partial dislocations. Normally such systems are observed in the [110] direction. By looking also at the [100] direction it has been found, that defects, which are clearly visible in one direction are nearly invisible in the other. This may lead to a misinterpretation of the structural perfection, if one considers only one direction.

HL 81.11 Thu 17:45 EW 201

Towards enhancement mode AlInN/AlN/GaN FETs using p-GaN cap layers — •Jonas Hennig, Armin Dadgar, Hartmut Witte, Juergen Blaesing, and Andre Strittmatter — Otto-von-Guericke Universität Magdeburg, Fakultät für Naturwissenschaften, Universitätsplatz 2, 39104 Magdeburg

With their large electric breakdown-field GaN based field effect transistors are ideally suited for high power electronics for voltages above 600 V and currents up to hundreds of amperes. The abrupt spontaneous polarization change at the AlInN/GaN heterojunction produces large sheet carrier concentrations, higher than for conventional AlGaN/GaN heterojunctions which results in a highly conductive channel even without bias. For safety reasons, however, these devices are required to operate in normally-off mode. By introducing a magnesium doped GaN cap layer on top of the AlInN the resulting electric field may deplete the channel under the gate region from charge carriers at zero gate bias. We currently conduct studies on p-GaN/AlInN/AlN/GaN FET structures grown on Si (111) by MOVPE and will present first results on the impact on FET performance. The analyses are carried out by XRD, AFM, Hall-effect, and current-voltage measurements.

HL 81.12 Thu 18:00 EW 201

Thermal and optical defect spectroscopy in AlInN/AlN/GaN hetero-structures on Si(111) — •Aqdas Fariza, Hartmut Witte, Jonas Hennig, Jürgen Bläsing, Armin Dadgar, Andre Strittmatter, and Alois Krost — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Magdeburg, Germany

AlInN/GaN based high electron mobility transistors (HEMTs) are ideally suited for high power applications because of high electron concentrations and mobility. Additionally, the growth of AlInN/GaN HEMTs on Si-substrates has many advantages to reduce device costs. But, the presence of defects and traps constitutes a major problem which leads to leakage currents and other degradation effects. Some traps have been assigned to cause these phenomena but still there is lacking information for structures on Si substrates. Temperature dependent I-V- and C-V-characteristics were carried out as well as thermal and optical admittance spectroscopy and photo-induced current transient spectroscopy for trap characterization both in InAlN/AlN/GaN/Si(111) hetero-structures and in GaN/Si(111) buffer layers. In both sample types identical trap emissions between 60 meV and 350 meV were found. All methods demonstrate strong optical quenching effects and non-shifting peak positions when changing the emission rates caused by the presence of mid gap traps in GaN. In contrast, the InAlN layers yield a shallow thermally activated resistivity up to 40 meV.