

HL 11 II-VI Halbleiter I

Zeit: Freitag 15:00–16:30

Raum: TU P164

HL 11.1 Fr 15:00 TU P164

Optische und strukturelle Eigenschaften von MgZnO/ZnO-Hetero- und -Doppelheterostrukturen — ●SUSANNE HEITSCH, GREGOR ZIMMERMANN, HOLGER HOCHMUTH, GABRIELE BENNDORF, HEIDEMARIE SCHMIDT, MICHAEL LORENZ und MARIUS GRUNDMANN — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstr. 5, D-04103 Leipzig

MgZnO-Dünnschichten, MgZnO/ZnO-Heterostrukturen und -Doppelheterostrukturen (DHS) wurden auf *a*-Saphir-Substraten mittels Pulsed Laser Deposition (PLD) abgeschieden. In Photolumineszenz (PL)-Untersuchungen bei 2 K beobachtet man eine Blauverschiebung der Bandlücke des MgZnO mit steigendem Mg-Gehalt. AFM-Untersuchungen zeigen die Rauigkeit der MgZnO-Barrierschichten auf, deuten jedoch auch auf ein gleichmäßiges Wachstum der ZnO-Schichten auf allen auftretenden Facetten des MgZnO hin. PL-Untersuchungen an Heterostrukturen beweisen die gute optische Qualität des auf MgZnO abgeschiedenen ZnO. Für MgZnO/ZnO/MgZnO-DHS mit nominellen Quantengrabbereitungen von ≤ 6 nm ist in PL-Spektren bei 2 K eine deutliche Intensivierung der vom ZnO herrührenden PL gegenüber dickeren DHS beobachtbar. Temperaturabhängige Messungen zwischen 4.4 und 300 K zeigen, dass die dabei dominierende Rekombination freien Exzitonen zuzuschreiben ist, deren Emissionsenergie durch Confinement-Effekte um bis zu 50 meV gegenüber Bulk-Material blauverschoben ist.

HL 11.2 Fr 15:15 TU P164

Combining quasiparticle energy calculations with exact-exchange density-functional theory for II-VI compounds and group-III-nitrides — ●PATRICK RINKE¹, ABDALLAH QTEISH², JÖRG NEUGEBAUER³, CHRISTOPH FREYSOLDT¹, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — ²Department of Physics, Yarmouk University, Irbid - Jordan — ³Department of Theoretical Physics, University of Paderborn, Paderborn

We present a systematic *ab initio* study of the electronic structure for selected II-VI compounds and group III nitrides in the zinc-blende structure with special emphasis on the role played by the semicore *d*-electrons. We show that applying density-functional theory (DFT) in the exact-exchange (EXX) approach [1] leads to an improved description of the *d*-electron hybridisation compared to the local-density approximation (LDA). Moreover we find that it is essential to use the newly developed EXX pseudopotentials [2] in order to treat core-valence exchange consistently.

In combination with quasiparticle energy calculations in the *GW* approximation we achieve very good agreement with available photoemission data. Since the DFT energies and wavefunctions serve as input for the *GW* calculation we conclude that for these materials EXX constitutes the better groundstate.

[1] M. Städele *et al.*, Phys. Rev. Lett. **79** 2089 (1997)

[2] M. Moukara *et al.*, J. Phys.: Condens. Matter **12** 6783 (2000)

HL 11.3 Fr 15:30 TU P164

Quadrupole Interaction in Semiconductors with Wurtzite Lattice: DFT-Theory and Experiments — ●SEPP UNTERRICKER¹, VEACESLAV SAMOKHVALOV², FRANK SCHNEIDER¹ und MARC DIETRICH³ — ¹Institut für Angewandte Physik, TU Bergakademie Freiberg, D-09596 Freiberg — ²AMD Dresden — ³Deutsche Solar AG Freiberg

Quadrupole coupling constants as determined by methods like NMR, Mössbauer spectroscopy and PAC (perturbed angular correlations) can be calculated by modern methods of solid state theory from the electronic charge density distribution. In the presented contribution binary semiconductors with wurtzite structure are investigated. The calculations were performed with the WIEN97 code. In a first step accurate displacement parameters *u* were determined by the minima of total energies and the zero crossing of atomic forces. For host probes the theoretical electric field gradients reflect the experiments well. Especially by the PAC-method cases with impurity probes, e.g. doping atoms, can be measured also. The calculation of such configurations is more expensive because the elementary cell has to be enlarged and atomic relaxations to be considered.

HL 11.4 Fr 15:45 TU P164

Whispering Gallery Moden in hexagonalen Zinkoxid Mikro- und Nanoresonatoren — TH. NOBIS, A. RAHM, E. M. KAIASHEV, M. LORENZ, M. GRUNDMANN, ●TH. NOBIS, A. RAHM, E. M. KAIASHEV, M. LORENZ und M. GRUNDMANN — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Linnéstr. 5, D-04103 Leipzig

In den vergangenen Jahren wurden Whispering Gallery Resonatoren, in deren Innern das Licht durch Totalreflexion umläuft, intensiv untersucht. Deren typische laterale Abmessungen liegen im Mikoregime bei $D \gg 1 \mu\text{m}$. Die Nanophotonik erfordert jedoch immer kleinere Kavitäten. Deshalb präsentieren wir in diesem Beitrag orts- und polarisationsabhängige Lumineszenzuntersuchungen an hexagonalen Zinkoxidsäulen und -nadeln, deren Dimensionen bis zu $D \simeq \lambda/n \simeq 200$ nm reichen. Die für ZnO-Bulkmaterial typische grüne Lumineszenz der Nanokristalle weist hierbei charakteristische Peakserien auf. Mittels eines einfachen Ebene-Wellen-Modells können diese Peakserien durch Whispering Gallery Moden (WGM) eines hexagonalen Resonators erklärt werden. Ferner kann an einer einzelnen ZnO Nanonadel systematisch die Blauverschiebung der WGM bei kleiner werdenden Resonatordurchmessern beobachtet und somit direkt der Übergang vom Mikro- ins Nanoregime verfolgt werden. Beim Annähern an die Nadelspitze erkennt man die Anregung von WGM bis zur Modenzahl $N = 1$.

HL 11.5 Fr 16:00 TU P164

Empirical Pseudopotential Calculation of $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ ($0 \leq x \leq 1$) — ●DANIEL FRITSCH, HEIDEMARIE SCHMIDT, RÜDIGER SCHMIDTGRUND, and MARIUS GRUNDMANN — Universität Leipzig, Fakultät für Physik und Geowissenschaften

We have investigated the electronic properties of the ternary alloy $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ ($0 \leq x \leq 1$) by means of the Empirical Pseudopotential Method (EPM). Making use of transferable ionic model potential parameters we obtained the band dispersions of wurtzite ZnO and rocksalt MgO that compare to low-temperature experimental data, thereby validating the transferability of the used EPM parameters. Those transferable parameters are a good starting point for EPM calculations of the ternary alloy ZnMgO by means of the Virtual Crystal Approximation (VCA). We present the calculated band structures of $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ for $0 \leq x \leq 1$ where the alloy dependent crystal modification is wurtzite for $x \leq 0.6$ and rocksalt for $x \geq 0.7$. For a better comparison with room-temperature experimental studies we weighted the EPM parameters with temperature dependent Debye-Waller factors by means of a model introduced by Brooks and Yu.

The obtained room-temperature band structures are discussed with respect to electronic band-to-band transitions leading to critical points in the dielectric function of $\text{Zn}_{1-x}\text{Mg}_x\text{O}$ measured by spectroscopic ellipsometry in the energy range from 0.75 eV up to 9 eV.

HL 11.6 Fr 16:15 TU P164

First-Principles Study on the Role of Oxygen Interstitials in Zinc Oxide — ●PAUL ERHART, KARSTEN ALBE, and ANDREAS KLEIN — TU Darmstadt, Institut für Materialwissenschaft, Petersenstraße 23, 64287 Darmstadt

The electronic and optic properties of zinc oxide are to a large extent controlled by intrinsic and extrinsic defects. Therefore, a detailed understanding of its defect physics is essential for successful defect engineering. In the past a number of first-principles studies has dealt with intrinsic point defects in zinc oxide. While these studies have essentially confirmed the importance of oxygen vacancies and zinc interstitials, the role of oxygen interstitials has been insufficiently explored. We have performed a careful study of numerous oxygen interstitial configurations based on density-functional theory calculations within the local density approximation. The charge state determines which configuration is energetically preferred: (1) if the defect is negatively charged, the most stable conformation is a split-interstitial which can be regarded as a strongly distorted tetrahedral interstitials; (2) on the other hand, if the oxygen interstitial is neutral or positively charged it assumes a dumbbell-like configuration in which two oxygen atoms share a site. This defect is characterized by a strong oxygen-oxygen bond which gives rise to its particular stability. Thanks to the oxygen-dimer-like structure it is able to compensate positive surplus charges in a manner that its formation energy remains almost constant as its charge state changes from neutral to doubly positive and

thus is a potential donor under oxygen-rich conditions.