HL 114: Oxides: Bulk, films and interfaces

Time: Friday 9:30–12:45 Location: POT 251

HL 114.1 Fri 9:30 POT 251

Structural and Electronic Properties of Si/ZnO Interfaces from ab-initio Quasiparticle Calculations — •Benjamin Höffling and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

Transparent conducting oxides like ZnO are widely used in Si-based photovoltaics. The fundamental properties of the Si/ZnO interface, however, remain poorly understood. We have employed Density Functional Theory and modern many-body perturbation theory using nonlocal exchange-correlation functionals and Hedin's GW method to a model interface derived from lattice coincidence considerations and the minimization of dangling bonds. We present results describing the atomic structure, electronic band offsets, interface states and the influence of passivation at the interface. We also discuss how band offsets derived from mesoscopic alignment methods like the Shockley-Anderson model or Tersoff's branch point method compare to the microscopic results.

HL 114.2 Fri 9:45 POT 251

Response of titanium dioxide after fs-laser excitation using ab-initio MD-simulations — •Sergej Krylow, Fairoja Cheenicode Kabeer, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretical Physics, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

We determined the response of titanium dioxide supercells using our in-house Code for Highly-excIted Valence Electron Systems(CHIVES), which is an implementation of electronic temperature dependent density functional theory using pseudopotentials and localized atom-centered basis functions. In particular, we are interested in the decay of the A1g-phonon mode as a function of time as well as the phonon-phonon interactions, which are causing the decay. We demonstrate that there is a dependence of the dynamics on the applied fs-laser laser fluence. We also compare our results to recent experiments[1], showing the accuracy of CHIVES.

[1] Bothschafter, E. M. and Paarmann, A. and Zijlstra, E. S. and Karpowicz, N. and Garcia, M. E. and Kienberger, R. and Ernstorfer, R: Ultrafast Evolution of the Excited-State Potential Energy Surface of TiO_2 Single Crystals Induced by Carrier Cooling, Phys. Rev. Lett. 110, 067402 (2013)

HL 114.3 Fri 10:00 POT 251

Diameter-dependent Absorption Edges of One-dimensional TiO2 Nanotube Arrays by Atomic Layer Deposition — •Ahmed Al-Haddad[1,2], Samar Tarish[1,2], Ranjith Vellacheri[1], Wenxin Wang[1], Fabian Grote[1], Zhibing Zhan[1], and Yong Lei[1] — [1]Ilmenau University of Technology, Institute of Physics & IMN MacroNano (ZIK) Prof. Schmidt-Str. 26, 98693 Ilmena,Germany. — [2]Department of Physics, College of Science, The University of Mustansiryah, Baghdad, Iraq.

Free standing one-dimensional (1-D) TiO2 nanotube arrays (TNAs) were fabricated by atomic layer deposition (ALD) with the assistant of anodic aluminum oxide templates at 350 °C. The wall thickness of nanotubes can be precisely controlled using ALD recipe. The intensities of the UV-Vis absorption were enhanced with increasing the diameter of nanotube while the thickness of the nanotubes walls was kept constant. A blue-shift was observed when decreasing the diameter of nanotubes, indicating a change of band gap and the shift of absorption edges towards shorter wavelengths were ascribed to the quantum effect of nanotube wall. Furthermore, the structure and surface morphology of the TNAs were examined by Raman spectroscopy and scanning electron microscopy, respectively.

HL 114.4 Fri 10:15 POT 251

Heteroepitaxial ZnO films on diamond — Fabian Schuster[1], •Martin Hetzl[1], Cesar Magén[2,3], Jordi Arbiol[4,5], Jose Garrido[1] und Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Laboratorio de Microscopías Avanzadas (LMA) - Instituto de Nanociencia de Aragon (INA) and Departamento de Física de la Materia Condensada, Universidad de Zaragoza, Spain — [3]Fundación ARAID, Zaragoza, Spain — [4]Institut de Ciència de Materials de Barcelona, ICMAB-CSIC, Bellaterra, Spain — [5]Institució Catalana de Recerca i Estudis Avancats (ICREA), Barcelona, Spain

The growth of heteroepitaxial ZnO films on (110) diamond substrates is demonstrated by molecular beam epitaxy. Structural characterization is performed by means of X-ray diffraction and scanning transmission electron microscopy imaging (STEM), where single domain growth is observed. The growth direction is found to be along the polar c-axis with Zn-polarity, deduced from annular bright field STEM. Photoluminescence and absorption studies reveal good optical properties as well as amplified spontaneous emission for optical excitation above a threshold of 30 kW/cm2. In addition, electronic band structure simulations are presented, showing that the ZnO polarity dominates the electronic structure of the interface: the formation of a 2DEG on the ZnO side or a 2DHG on the diamond side are predicted for Zn- and O-polarity, respectively.

HL 114.5 Fri 10:30 POT 251

A comprehensive study on ion-implantation induced defects in ZnO thin films — •Florian Schmidt[1], Stefan Müller[1], Holger von Wenckstern[1], Robert Röder[2], Sebastian Geburt[2], Carsten Ronning[2], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — [2]Friedrich-Schiller-Universität Jena, Institute for Solid State Physics, D-07743 Jena

Deep defects levels in semiconductors have significant impact on material properties and device performance. Therefore a profound understanding of such defects is helpful for device optimization. Devices based on the semiconductor ZnO has been reported in the last years and even simple transparent circuitry have been demonstrated [1].

Here we present characterization of deep-level defects introduced by implantation of Ar^+, Ne^+, Zn^- and O^- by means of deep-level transient spectroscopy (DLTS) and optical DLTS (ODLTS). Independent of the implanted ion defect levels with thermal activation energies of $E_a \approx 1000\,\text{meV}$ and $\approx 1200\,\text{meV}$ were introduced. A defect level with the thermal activation energy of 388 meV was only detectable after oxygen ion implantation. We will present for each ion implanted the density of the defects introduced.

[1] H. Frenzel *et al.*, phys. stat. sol. RRL **7** (9), 605 (2013).

HL 114.6 Fri 10:45 POT 251

Influence of deposition parameters on *p*-NiO/*n*-ZnO heterojunctions — •Paul Räcke, Robert Karsthof, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig, Germany

An ideal transparent solar cell completely transmits the visible part of the solar spectrum. At the same time, the energy of the rest of the solar spectrum is converted into electric power as efficiently as possible. A few wide-gap transparent semiconductors are candidates for the construction of a photovoltaic cell that absorbs radiation in the UV spectral range.

In this work the optical and electrical properties of zinc oxide-nickel oxide thin film heterojunctions were studied. The *p*-type NiO was grown by reactive DC sputter deposition onto pulsed laser deposited (PLD) *n*-type ZnO with a highly transparent ZnO:Al back contact on *a*-sapphire. A very thin gold layer on top of the NiO works as hole extraction layer. The result is a semi-transparent cell stack for which the transmission is mainly limited by the NiO layer and depends on its thickness and stoichiometry.

We investigated the influence of the NiO film thickness on the transmission spectrum and the IV characterstics including photovoltaic parameters. Furthermore, the transmission by the NiO was improved tremendously by annealing the cell stack in an oxygen ambient. The changes in the IV characteristics will be discussed as well.

Coffee break (15 min.)

HL 114.7 Fri 11:15 POT 251

Formation of stable bound magnetic polarons in depleted ZnCoO films — •T. Kaspar[1], D. Bürger[1], I. Skorupa[2], O.G. Schmidt[1,3], and H. Schmidt[1] — [1]TU Chemnitz, 09111 Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden,

Germany — [3]IFW Dresden, 01069 Dresden, Germany

Metal-semiconductor field effect transistors (MESFET) with a paramagnetic ZnCoO [1] channel and a free charge carrier concentration below the metal insulator transition [2] have been fabricated by pulsed laser deposition on c-plane sapphire substrates. The unstructured ZnCoO films reveal a positive magnetoresistance due to s-d- exchange interaction effects. We show that the formation of stable BMPs with a stable defect [3] is responsible for switching depleted ZnCoO from a low into a high resistance state by applying an external magnetic field. The high resistance state is persistent until the MESFET is heated up to 300 K and is caused by the formation of stable bound magnetic polarons (BMPs) in depleted ZnCoO. This effect could be possibly used for the realization of nonvolatile spin valves in ZnCoO films with two gate contacts. [1] T. Kaspar et al., IEEE 34, 1271 (2013) [2] Q.Y. Xu et al., J. Appl. Phys. D-Appl. Phys. 42, 085001 (2009); Phys. Rev. B 73, 205342 (2006); Phys. Rev. B. 76, 134417 (2007) [3] H. Schmidt et al., Appl. Phys. Lett. 91, 232110 (2007).

HL 114.8 Fri 11:30 POT 251

Structure dependent magnetic properties of Co implanted TiO2 — •Oguz Yildirim[1,2], Steffen Cornelius[1], Maik Butterling[3], Wolfgang Amwand[3], Andreas Wagner[3], Alevtina Smekhova[4], and Kay Potzger[1] — [1]Institute for Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Institute for Physics of Solids, TU Dresden, Zellescher Weg 16, 01069 Dresden, Germany — [3]Institute for Radiation Physics , HZDR, Dresden, Germany — [4]Lomonosov Moscow State University, MSU, Faculty of Physics, Moscow, Russia

Magnetic and structural properties of amorphous and anatase TiO2 thin films implanted with Co ions have been investigated. Implantation induced defects have been characterized using positron annihilation spectroscopy (PAS) while for magnetic chracterization we have used magnetometry. Up to a doping level of 2.5 at.%, only a paramagnetic contribution has been detected. The susceptibility strength , however, depends on the structure of the unimplanted film. Results on the formation of secondary phases at higher doping level will also be presented.

This work is supported by the Initiative and Networking Fund of the German Helmholtz Association, Helmholtz-Russia Joint Research Group HRJRG-314, and the Russian Foundation for Basic Research, RFBR 12-02-91321-SIG, Start: 01.02.2012

HL 114.9 Fri 11:45 POT 251

Multicentric coordination of hydrogen in the metal oxides ZnO and MgO — •Sandro G. Koch, Edward V. Lavrov, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

Hydrogen is an inherent impurity in ZnO and MgO. The formation of shallow hydrogen donors and the passivation of acceptors as well as F-centers significantly influence the optical and electrical properties of these materials. Calculations by Janotti and Van de Walle suggested that hydrogen substituting for oxygen (H_O) in ZnO and MgO binds equally to all metal neighbors resulting in a lower local vibrational mode (LVM) frequency compared to a two-center bond. The authors introduced the concept of the hydrogen multicenter bond in solids to visualize their results [1]. An experimental verification of this hypothesis is challenging, since the predicted LVM frequencies are located in a multi-phonon absorption region.

Here, we present an experimental approach to overcome the LVM detection limitation in strongly absorbing spectral regions. Using the photoconductivity technique we show that H_O in ZnO is tetrahedrally coordinated with LVMs at 742 and 792 cm^{-1} [2]. First preliminary results on H_O in MgO are also presented .

[1] A. Janotti and C. Van de Walle, Nat. Mater. **6**, 44 (2007).
[2] S. G. Koch *et al.*, Phys. Rev. Lett. **108**, 165501 (2012).

HL 114.10 Fri 12:00 POT 251

Recharging behaviour of nitrogen-centers in ZnO — •Jan M. Philipps[1], Bruno K. Meyer[1], Detlev M. Hofmann[1], and Matt McCluskey[2] — [1]Institute of Physics I, Heinrich-Buff-Ring 16, Justus-Liebig-University Giessen, D-35392 Giessen, Germany — [2]Department of Physics and Astronomy, Washington State University, Pullman, WA 99164-2814, USA

Nitrogen was quoted to be a candidate to obtain p-type conductive ZnO. One assumes in a simple model that nitrogen substitutes an oxygen atom in the crystal lattice and thus causes an acceptor. The hope was that the recharging level of the nitrogen acceptors is shallow enough to accept electrons from the valence band and thus to promote hole conductivity. Unfortunately, it turned out that this model was too simple, electron paramagnetic resonance experiments (EPR) revealed that substitutional nitrogen centers (N_O) are deep defects with a recharging level 1.3 eV above the valence band.

In the following it was speculated that nitrogen-pair centers or complexes consisting of nitrogen and vacancies could act as shallow acceptors. Again EPR was successful to identify N_2-centers in ZnO by the observation of a 5-line spectrum caused by the hyperfine interaction of two nitrogen nuclei. The recharging of this center exhibits two steps, a weak onset at about 1.4 eV and a strongly increasing signal for photon energies above 2.1 eV. The later energy coincides with the recharging energy of the N_O-centers. These results indicate that also the N_2-centers are deep level defects and not suitable to cause significant hole-conductivity at room temperature.

HL 114.11 Fri 12:15 POT 251

Highly rectifying contacts on amorphous zinc-tin-oxide thin films consisting of metals and p-type zinc-cobalt-oxide — •Peter Schlupp, Friedrich-Leonhard Schein, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Leipzig, Deutschland

In order to provide cost-efficient and homogeneous oxide thin films for electronic devices it is desirable to use amorphous materials which can be deposited at room temperature (RT). Zinc-tin-oxide (ZTO) is a promising *n*-type semiconducting material in which only abundent materials are contained. To produce MESFETs or JFETs highly rectifying Schottky contacts or *pn*-heterodiodes are needed. The latter could be realized with *p*-type semiconductors like zinc-cobalt-oxide (ZCO).

We present electrical properties of highly rectifying contacts on amorphous ZTO layers. Our first metal-semiconductor structures showed only weakly rectifying behavior due to trap-assisted tunnel currents. In order to improve rectification, we introduced a thin insulating ZTO layer between the metal and the thin film. Optimized Schottky contacts on this structure exhibit current on/off-ratios up to 10^7 at ± 2 V. Using p-type ZCO we fabricated all-amorphous oxide heterodiodes. Again, we introduced an insulating ZTO layer on the *n*-side of the heterointerface and obtained *pin*-diodes having current on/off ratios up to 5×10^6 at ± 1.6 V. Thus they widely outperform the previously best fully amorphous TSO *pn*-junctions. Temperature dependent current-voltage characteristics and the current transport mechanism across the heterointerface will be discussed.

HL 114.12 Fri 12:30 POT 251

Transparent photovoltaics: ZnO/NiO heterojunctions working as UV solar cells — •Robert Karsthof, Paul Räcke, Zhipeng Zhang, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Insitut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig, Germany

A solar cell transmitting visible light rather than absorbing it seems to contradict the general idea of efficient energy conversion. However, it has been shown recently [1] that a device which only absorbs photons from the IR and UV range of the solar spectrum can reach conversion efficiencies up to 37% (Shockley-Queisser limit). PV modules consisting of such cells could be used to generate electric power e.g. on large window areas on office buildings without reducing the daylight illumination of the interior – in contrast to conventional technologies.

In this work we present an approach based on zinc oxide-nickel oxide thin film heterojunctions. We grew *p*-type NiO by reactive DC and RF sputter deposition on top of pulsed laser deposited (PLD) *n*-type ZnO on *a*-sapphire to produce semi-transparent *pn*-junctions. A highly Al-doped PLD-grown ZnO layer was used as transparent back contact. The completed cell stack showed a high transmission of 50% and above. The cells were characterized by means of *IV* and external quantum efficiency (EQE) measurements. We could confirm that with this approach energy conversion efficiencies above 1% and EQE around 100% in the UV range are already feasible.

[1] R. Lunt: *Appl. Phys. Lett.* **101**, 043902 (2012)