HL 100: ZnO and its relatives

Time: Friday 9:30–12:15 Location: EW 203

HL 100.1 Fri 9:30 EW 203

First-principles Evidence for Intermediate Hole Polarons in ZnO — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[1,2], Matthias Scheffler[1], Hikmet Sezen[3], Fabian Bebensee[3], Chengwu Yang[3], Maria Buchholz[3], Alexei Nefedov[3], Stefan Heissler[3], and Christof Woell[3] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Aalto University, Helsinki, Fi — [3]Karlsruhe Institute of Technology, Karlsruhe, DE

We performed density functional theory calculations at the hybrid-functional level (HSE06) to investigate the nature of the polaronic states in ZnO. Our calculations confirm that neither small (i.e., strong coupling) electron nor hole polarons are stable in ZnO, in agreement with previous studies [1]. The binding energy of large polarons (i.e., weak coupling) was determined by evaluating the renormalization of the band edges due to the zero-point motion of the atoms [2]. However, for intermediate polarons at intermediate coupling strength, the harmonic approximation breaks down, and there is currently no first-principle theory. We use the HSE06 effective masses to calculate the Fröhlich coupling constants α. Feynman's path integral technique then yields an intermediate hole polaron, whose binding energy of 245 meV and associated peaks in the optical absorption spectrum are consistent with infrared reflection absorption spectroscopy. [1] J. B. Varley *et al.*, Phys. Rev. B **85**, 081109(R)(2012), [2] G. Antonius *et al.*, Phys. Rev. Lett. **112**, 215501 (2014)

HL 100.2 Fri 9:45 EW 203

Characterization of the p-GaAs / n-ZnO tunnel contact system for opto-electronic applications — •Christian Koppka, Andreas Nägelein, Katja Tonisch, and Thomas Hannappel — Technische Universität Ilmenau, FG Photovoltaik, 98693 Ilmenau, Deutschland

Nanowire based concepts for optoelectronic applications such as LEDs, sensors and solar cells are current global research areas. In contrast to axial structures, the front contacting of nanowire structures with radial configuration is more challenging. In this regard, we examine the contacting of p-doped GaAs nanowire shells using AlOx and ZnO:Al to realize a tunnel junction at the interface. To achieve a good contact system we investigate a ALD type growth of AlOx and ZnO:Al layers for the homogeneous coating of non-planar surfaces in a conventional MOCVD reactor (AIX 200). Due to the very limited analysis methods for coated nanowires structures, the characterization of the p-GaAs/AlOx/n-ZnO system was carried out on planar samples. Current-voltage measurements reveal an ohmic behavior between TCO and III-V material and confirm the applicability of the contact system. By depth-resolved auger electron spectroscopy measurements no diffusion processes of Al or As were found. Accordingly, a sharp interface is assumed. Our ALD process was used successful on nanowire structures and reveal a homogeneous coating.

HL 100.3 Fri 10:00 EW 203

Low temperature PLD-growth of ZnO nanowires on $Zn_xAl_{1-x}O$ films — •Alexander Shkurmanov, Chris Sturm, Helena Franke, Holger Hochmuth, and Marius Grundmann — Inst. f. Exp. Phy. II, Universität Leipzig, Leipzig, Germany

Self-organized grown ZnO micro- and nanostructures exhibit high crystallinity and good electronic properties which makes them interesting to be implemented in devices. In order to integrate these nanostructures in CMOS technology, a growth temperature of less than 450°C is required. For nanowires (NW) prepared by pulsed laser deposition (PLD) typically temperatures of about 900°C are used [1] and a reduction of temperature is quite challenging. In this work, we present the impact of the Al concentration of the ZnO seed layer on the NW growth and as a function of temperature in the range from 400°C to 950°C. At high temperatures (950°C), the Al concentration has a strong influence on the morphology of the NWs as well as on the NW density. The highest NW density we observed for an Al concentration of about 1.5% within the seed layer whereas for larger values, no NW growth was observed. By reducing the temperature down to 400°C a decrease of the density and length of NWs can be observed. This can be attributed to the reduced surface mobility of the incoming particles due to the reduced temperature and a possible change of the polarity of the seed layer by the Al incorporation [2]. [1] C.P. Dietrich, M. Grundmann in *Wide Band Gap Semiconductor Nanowires 1*, V. Consonni, G. Feuillet eds., (Wiley-ISTE, 2014). [2] S. Käbisch et al., Appl. Phys. Let. **103**, 103106 (2013).

HL 100.4 Fri 10:15 EW 203

Influence of mechanical destruction on phonons and excitonic transition on polar and non-polar ZnO crystals — •Nadja Jankowski[1], Christian Nenstiel[1], Mark Berkahn[2], Matthew Phillips[2], and Axel Hoffmann[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]School of Physics and Advanced Materials, University of Technology, Sydney, Australia

As Zinc Oxide (ZnO) is a very soft material it is very sensitive towards destruction during handling, thus it is interesting to study the influence of mechanical destruction on optical and structural properties. Therefore polar (c-orientated) and non-polar (a- and m-orientated) ZnO crystals where locally destroyed with a spherical indenter with a diameter of 1 μm and an applied load of 100 mN.

The influence of the destructed area on strain fields and crystal quality was investigated in detail by the means of Raman map scans. The shift of the E_2^{high}-mode revealed complex strain fields with hexagonally arranged strain fields for the polar plane and elongated V-shaped bands of strain for the non-polar plains.

The influence on the excitonic recombination due to destruction was investigated by micro photoluminescence at about 10 K. In general the excitonic transition shows a shift according to the strain fields. On the non-polar planes a change of the intensity ratio between high and low energy neutral bound excitons and the ionized bound ones can be observed in the compressive and tensile strained regions. Therefore a clear connection between the change of excitonic transition and the indentation induced strain fields can be observed.

HL 100.5 Fri 10:30 EW 203

Room-temperature fabricated amorphous oxide heterodiodes on glass and flexible substrates — •Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für experimentelle Physik II, Leipzig, Germany

Beside the lower energy input, room-temperature (RT) fabrication of semiconductors has the advantage that thermally unstable but flexible substrates can be used. The amorphous oxides *n*-type zinc-tin oxide (ZTO) and *p*-type zinc-cobalt oxide (ZCO) show promising semiconducting properties even though they are fabricated at RT [1,2]. Furthermore they contain abundant materials only.

We present electrical properties of ZTO/ZCO heterodiodes fabricated entirely at RT by pulsed laser deposition. These diodes were deposited on corning glass substrates and on flexible plastic substrates. To enhance the rectification of the diodes, an ultrathin insulating ZTO layer was introduced at the heterointerface leading to bipolar diodes with a rectification ration of more than six orders of magnitude. The diode properties and the conduction mechanism will be derived from temperature dependend current voltage measurements. Furthermore we have investigated the influence of bending of the flexible substrates on the diode properties.

[1] Schlupp et al., MRS Proceedings **1633**, 101 (2014)
[2] Schein et al., Appl. Phys. Lett., **104**, 022104 (2014)

Coffee break

HL 100.6 Fri 11:00 EW 203

Selective Back Channel Passivation of ZnO TFTs Utilizing Oxiranes — •Marlis Ortel, Nataliya Kalinovich, Gerd-Volker Röschenthaler, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Zinc oxide layers of 10nm film thickness were deposited by spray pyrolysis as active layer in TFT structures. They were utilized to investigate the influence of the surface at the back channel on the charge transport processes in ZnO TFTs by detailed IV analysis. A strong but reversible increase of shallow and deep trap states was found when the material was exposed to humid atmosphere. This results in a decrease in mobility, increase in hysteresis and shift of the threshold voltage during gate bias stress due to coulomb interaction of surface and active channel charges.

Oxiranes were selectively bound to hydroxyl groups at the metal oxide surface to gain information about the active sides at the surface which induce the change of the electronic surface structure. The binding of hexafluoropropylene oxide self-assembled monolayer (SAM) to the surface caused a significant decrease in hysteresis by a factor of 4. Furthermore, no shift of the on-set under negative gate bias stress was observed after oxirane treatment and the mobility remained stable. We conclude that hydroxyl surface groups act as active sides to induce mainly deep trap levels at the back channel of ZnO TFTs in humid atmosphere.

HL 100.7 Fri 11:15 EW 203

Blue shifting the photoluminescence of ZnO by doping with amino acids — •Marlene Lamers[1,3], Verena Baumann[1,3], Anastasia Brif[2], Guy Ankonina[4], Alexander Urban[1,3], Jessica Rodríguez-Fernández[1,3], Boaz Pokroy[2], and Jochen Feldmann[1,3] — [1]Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität, Munich — [2]Department of Materials Science and Engineering and the Russell Berrie Nanotechnology Institute of Technology, Haifa, Israel — [3]Nanosystems Initiative Munich (NIM), Munich — [4]Photovoltaic lab, Department of Electrical Engineering, Technion Israel Institute of Technology, Haifa, Israel

Zinc oxide (ZnO) is an attractive semiconductor due to its wide and direct bandgap in the UV region (Eg = 3.4 eV), its large free-exciton binding energy (60 meV) and its strong photoluminescence even at room temperature. Bandgap tuning is of special interest to extend the spectral range of ZnO based devices. Recently, it has been demonstrated by optical reflection spectroscopy that the bandgap of zinc oxide can be engineered by intracrystalline incorporation of amino acids due to an increased lattice strain [1]. We have performed photoluminescence and absorption experiments, which reveal a controlled blueshift of the bandgap emission for amino acid doped ZnO vs. pure ZnO. Additionally, the ratio of band-edge-to-defect emission can be significantly enhanced by post-synthetic heat treatment. Morphological changes will be discussed as a possible reason for these observations.

[1] A. Brif, G. Ankonina, C. Drathen, B. Pokroy, Adv. Mater. (2014) 26, 477.

HL 100.8 Fri 11:30 EW 203

Influence of Fe impurities on the annealing of OH-Li complexes in ZnO — •Frank Herklotz, Klaus Magnus Johansen, Augustinas Galeckas, and Bengt Gunnar Svensson — University of Oslo, Department of Physics/Centre for Materials Science and Nanotechnology, N-0318 Oslo, Norway

The annealing behavior of the OH-Li_{Zn} center in ZnO, which leads to a local vibrational mode at 3577 cm^{-1}, has been studied. Infrared absorption measurements confirm the previous findings that the center dissociates already at about 450 °C and an apparent stability up to 1250 °C is due to efficient retrapping of H by Li_{Zn}. Secondary ion mass spectrometry data strongly indicate that Fe impurities prevent a reformation of OH-Li_{Zn} after dissociation. The formation of Fe-Li complexes is proposed as a mechanism for this behavior. Absorption lines due to Fe in as-grown and intentionally doped ZnO crystals are studied.

HL 100.9 Fri 11:45 EW 203

Effects of the growth temperature on the properties of RF sputtered $Zn_{1-x}Mg_xO$:Al thin films — •Philipp Schurig[1], Benedikt Kramm[1], Shengqiang Zhou[2], Angelika Polity[1], and Bruno K. Meyer[1] — [1]1. Physikalisches Insitut, Justus-Liebig-Universität Giessen, Deutschland — [2]Functional Materials, Helmholtz-Zentrum Dresden-Rossendorf, Germany

Transparent conductive materials (TCMs) are of major interest for optoelectronic or photovoltaic applications, i.e. ZnMgO:Al can be used as a window layer material or transparent electrode in solar cell applications. ZnMgO:Al can be tuned by variation of the magnesium content concerning the band gap or electrical properties, respectively. The thin films were deposited by RF sputtering on c sapphire and soda lime glass substrates. A ceramic ZnMgO:Al target was used as sputtering source.

The influence of the growth temperature on the structural, optical and electrical properties is investigated using various methods, e.g. XRD, SEM, XPS, UV-Vis NIR and Hall measurements. With increasing growth temperature the structure of the films changes from wurzite (low temp.) to rock salt-phase (high temp.), whereas the wurzite phase was the main interest in this research. With higher temperatures the ZnO (0 0 2) diffraction peak shifts to higher angles which indicates a higher magnesium content. The band gap also shifts to higher values, from 3.9 to 4.1 eV. The growth temperature influence on the electrical properties couldn't be determined, because other aspects do influence these as well, e.g. the grain size or the Mg content, respectively.

HL 100.10 Fri 12:00 EW 203

The influence of Al and Ga dopants on the structural, electrical and optical properties of (Mg,Zn)O thin films grown by PLD — •Abdurashid Mavlonov, Steffen Richter, Holger von Wenckstern, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

We have investigated structural, electrical and optical properties of Al- and Ga-doped (Mg,Zn)O thin films in dependence on the doping and alloy concentration. For this purpose, the samples have been prepared with two perpendicular, lateral composition gradients (Mg composition is varied in one direction whereas the Al/Ga concentration is varied in a perpendicular direction) [1]. The thin films were grown by pulsed-laser deposition (PLD) using a threefold segmented PLD target, a growth temperature of 600°C and 2-inch in diameter $c-$plane sapphire substrates. With increasing free charge carrier concentration N_{Hall} in a range from 1×10^{19} to 3×10^{20} cm^{-3}, the dielectric functions (DF) of the films show drastic changes due to increased (a) free-carrier absorption in the infrared region and (b) the Burstein-Moss effect in the ultraviolet region [2]. It has been found that the dopant efficiency and mobility tend to decrease with increasing Mg content, showing significant dependence in the case of Ga-doped films which can be explained with increasing the density of acceptor like compensating defects.

[1] H. von Wenckstern *et al.*: CrystEngComm 15, 10020 (2013).
[2] H. Fujiwara and M. Kondo, PRB 71, 075109 (2005).