HL 27: Zinc Oxide and Zinc Selenide

Time: Tuesday 9:30–13:00 Location: H17

HL 27.1 Tue 9:30 H17

Self-compensation in Al and Ga doped (Mg,Zn)O PLD thin films — •Abdurashid Mavlonov, Steffen Richter, Holger von Wenckstern, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Leipzig, Germany

The Al and Ga doping efficiency of transparent conductive (Mg,Zn)O thin films has been investigated in dependence on growth and annealing parameters. For this purpose, the samples have been prepared on glass substrates at RT, 200 °C, and 300 °C by pulsed-laser deposition (PLD) using a continuous composition spread method (CCS) [1, 2]. Further, post-annealing was performed at 400 °C in vacuum in order to analyze the stability of the films. It has been found that growth and annealing conditions have an impact on structural, electrical, and optical properties of the films. With increasing growth temperature, crystallographic quality of the films improved. However, at high temperature, i.e. after post-annealing at 400 °C, the free charge carrier density saturated and optical bandgap decreased. That can be explained by self-compensation of free charge carriers by intrinsic defects [2, 3].

[1] H. von Wenckstern *et al.*, CrystEngComm **15**, 10020 (2013).
[2] A. Mavlonov *et al.*, PSS-A 2015, DOI:10.1002/pssa.201431932.
[3] A. Zakutayev *et al.*, APL **103**, 212306 (2013).

HL 27.2 Tue 9:45 H17

Hybrid top gate transistors based on solution processed Zinc Tin Oxide and organic dielectrics — •Benedikt Sykora and Heinz von Seggern — TU Darmstadt, Materialwissenschaften, Elektronische Materialeigenschaften, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany

Metal oxide semiconductors like Zinc Tin Oxide (ZTO) are extensively studied because of their solution processability, transparency and cost efficiency. Transistors with top contact configuration are widely reported in literature. Top gate transistors on the contrary have several advantages e.g. protection of semiconducting layer, switching speed.

Here we present hybrid inorganic-organic top-gate transistors based on solution processed ZTO and organic dielectrics. An ethanol based precursor solution route for ZTO was developed that is environmental friendly, cost efficient, simple to process and long term stable. Thin films are investigated by TEM, SEM, XPS, XRD and absorption measurements. Transparent, top gate transistors exhibiting electron mobility values of up to 2.8 $cm^2/(Vs)$ and high on/off ratios exceeding 10^6 were realized.

HL 27.3 Tue 10:00 H17

CMOS-compatible PLD-growth of ultrathin ZnO nanowires — •Alexander Shkurmanov, Chris Sturm, Holger Hochmuth, and Marius Grundmann — Universität Leipzig, Inst. for Exp. Phys. II, Linnéstr. 5, 04103 Leipzig, Germany

An interesting feature of ZnO is self-organized growth of micro- and nanowires (NWs) with high crystalline quality. Comparing to microwires, quantum confinement effects appear in NWs with diameter less than 10 nm. This makes them interesting for quantum effects researches such as topological quibits [1].

Here we present the growth of an array of well oriented ZnO NWs by pulsed laser deposition (PLD). For the NWs growth we used ZnO seed layers which are doped with Al or rather Ga. In dependence on the concentration of these metals in the seed layer we were able to change the diameter of these wires, by two orders of magnitude, i.e from d $\geq$ 550 nm down to 10nm. The aspect ratio for all wires is typically 70. Beside the shape of the wire, the seed layer has also an impact on the optimum growth temperature of the NWs which can be reduced down to 400°C, making them compatible with CMOS technology.

[1] S. Nadj-Perge, et al, Nature 468 (7327),1084, 2010.

HL 27.4 Tue 10:15 H17

Self-consistent hybrid functional calculations: Implications for structural and electronic properties of oxide semiconductors — •Daniel Fritsch, Benjamin Morgan, and Aron Walsh — Department of Chemistry, University of Bath, Claverton Down, BA2 7AY Bath, UK

Density functional theory has proven hugely successful in the calculation of structural properties of condensed matter systems and the electronic properties of simple metals. Band gaps of semiconductors and insulators, however, are often severely underestimated due to the limitations of existing approximate exchange-correlation functionals. Considerable improvements are possible by including a fraction of Hartree-Fock exchange, constructing a so-called "hybrid" functional. The precise proportion of Hartree-Fock exchange is typically treated as an empirical parameter chosen from intuition and experimental calibration.

This empirism can be removed with a recent self-consistent hybrid functional for condensed systems [1], which offers a new approach for parameter-free hybrid functional investigations. Using this approach, we report on the implications for structural and electronic properties of oxide semiconductors, with ZnO, SnO_2, and MgO as specific examples. Structural and electronic properties will be compared to theoretical and experimental data, showing considerable improvement with respect to previous approaches.

[1] J. H. Skone *et al.*, Phys. Rev. B **89**, 195112 (2014).

HL 27.5 Tue 10:30 H17

Mechanisms for p-type conduction in ZnO, (Zn,Mg)O, and related oxide semiconductors — •Daniel F. Urban, Wolfgang Körner, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

Intrinsically n-type oxide semiconductors like ZnO and (Zn,Mg)O can be turned into p-type materials if a sufficient amount of shallow acceptor defect levels in the band gap is created and a depletion of the net electron concentration which activates the acceptor levels is achieved. Motivated by recent experiments [1,2] on (Zn,Mg)O doped with nitrogen we analyze the defect levels of substitutional nitrogen (N_O), zinc vacancies (v_Zn) and their combination by means of self-interaction-corrected density functional theory calculations. We show how the interplay of defects can lead to the favoured shallow acceptor defect levels, although the levels of isolated point defects N_O lie too deep in the band gap for being responsible for p-conduction. We relate our results to p-type channels seen in polycrystalline ZnO containing grain boundaries [3] which allows us to develop an understanding of p-type mechanisms in ZnO, (Zn,Mg)O, and related materials.

[1] L. Liu, J. Xu, et al, Phys. Rev. Lett. 108, 215501 (2012).
[2] M. N. Amini, et al, Phys. Chem. 17, 5485 (2015).
[3] W. Körner and C. Elsässer, Phys. Rev. B 81, 085324 (2010).

HL 27.6 Tue 10:45 H17

Optimization of seed layer thickness to grow ZnO nanowires for hybrid solar cell applications — •Emily Tansey[1], Alejandra Castro-Carranza[1], Stephanie Bley[1], Jairo C. Nolasco[2], Tobias Voss[3], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen — [2]Energy and Semiconductor Research Laboratory, Carl von Ossietzky University of Oldenburg, 26129 Oldenburg — [3]Institute of Semiconductor Technology, TU Braunschweig University of Technology, 38092 Braunschweig

An interesting application of ZnO nanowires is the formation of hybrid junctions with other materials, e.g. polymers, to create solar cells. Wet chemical growth of ZnO nanowires is a low-cost method that implements zinc acetate hexahydrate in solution as a seed layer to form ordered nanostructures on metal oxide substrates. The current-voltage characteristics of this junction, however, show the formation of an unwanted potential barrier at the interface between the ordered nanowires and bottom oxide electrode, which must be considered to get efficient cells. To better understand the impact of the seed layer on this junction, its thickness is modified. Our results indicate that a thicker seed layer yields a higher potential barrier formed at the ZnO nanowires-metal interface. An optimal seed layer thickness for solar cell applications is proposed accordingly.

30 min. Coffee Break

HL 27.7 Tue 11:30 H17

Inversion of absorption anisotropy in wurtzite MgZnO — •Maciej Neumann[1], Martin Feneberg[2], Rüdiger Goldhahn[2], Jean-Michel Chauveau[3], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., 12489 Berlin, Germany — [2]Otto-von-Guericke-Universität Magdeburg,

39106 Magdeburg, Germany — [3]University of Nice Sophia-Antipolis, 06103 Nice, France

ZnO and its ternary alloy MgZnO are considered promising candidates for optoelectronic devices operating in the violet and ultraviolet regime. Therefore, the precise knowledge of its optical properties is mandatory. They are characterized by the dielectric function (DF) perpendicular and parallel to the optical axis, respectively.

Using spectroscopic ellipsometry the DFs were obtained from m-plane MgZnO thin films with Mg contents up to 45 %, grown on ZnO substrates by plasma-assisted molecular beam epitaxy. With increasing Mg content the absorption edges of the DFs shift to higher energies, whereas the splitting between the perpendicular and the parallel DF decreases. This results in an inversion of the absorption anisotropy above approximately 24 % Mg content. In order to gain insight this behavior a line shape analysis of the DFs in the vicinity of the bandgap is performed. It considers free excitons, exciton-phonon complexes, and Coulomb enhanced interband transitions, yielding characteristic transitions energies. Using these transition energies the inversion is explained in terms of valence band ordering and oscillator strength.

HL 27.8 Tue 11:45 H17

Schottky barrier diodes on amorphous zinc tin oxide — •Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Leipzig, Germany

Amorphous zinc tin oxide (ZTO) can be fabricated at room temperature and exhibits electron mobilities of more than $10\,cm^2V^{-1}s^{-1}$ [1]. This makes its use interesting for channel layers in pixel driving thin film transistors for active matrix displays. Schottky barrier diodes acting as gate are a viable option. They can additionally be employed for material characterization by space charge spectroscopy.

We present Schottky barrier diodes on ZTO using platinum contacts. The semiconducting films are grown by pulsed laser deposition, the Schottky contacts by reactive direct current sputtering. Diodes exhibit rectification ratios of more than 5 orders of magnitude. Temperature dependent current voltage characteristics were obtained and modelled using thermionic emission model. Additionally, capacitance-voltage and thermal admittance spectroscopy were performed. We found two defect levels in a-ZTO, one deep level at about 200 meV and one shallow level near the conduction band minimum who's properties are discussed following the method of Pautrat et al. [2].

[1] Jayaraj et al., J. Vac. Sci. Technol. B **26**, 495 (2008)
[2] Pautrat et al., Solid-State Electron. **23**, 1159 (1980)

HL 27.9 Tue 12:00 H17

Electron-hole recombination dynamics in CdS nanocrystals: limiting steps of photocatalytic H2 generation — •Thomas Simon, Michael Carlson, Jacek Stolarczyk, and Jochen Feldmann — Chair for Photonics and Optoelectronics Ludwig-Maximilians-Universität, Amalienstr. 54, 80799 Munich, Germany

Semiconductors functionalized with additional noble metal clusters are well-known materials for photocatalytic fuel generation. The generation of elemental hydrogen from aqueous solution with cadmium sulfide nanorods decorated with platinum particles is of particular interest. Here the photoexcited electron is efficiently transfered from the semiconductor to the metal where it in turn reduces water molecules to elemental hydrogen. However, the photohole is not able to oxidize the water molecules but has to be removed by a sacrificial reducing agent to prevent the crystal from oxidation [1]. We studied the relaxation and recombination pathways of photoexcited carriers by femtosecond transient absorption spectroscopy. We found that a non-perfect or unstable charge separation finally leads to enhanced electron-hole recombination diminishing the photocatalytic quantum yield. Proper deposition techniques of the co-catalyst particles can bypass this problem.

[1] T. Simon, N. Bouchonville, M.J. Berr, A. Vaneski, A. Adrović, D. Volbers, R. Wyrwich, M. Döblinger, A.S. Susha, A.L. Rogach, F. Jäckel, J.K. Stolarczyk and J. Feldmann Nat. Mat. 13, 1013-1018 (2014)

HL 27.10 Tue 12:15 H17

Magnetic-Field-Induced Second-Harmonic Generation in ZnSe — •Johannes Mund[1], Walter Warkentin[1], and Dmitri Yakovlev[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

We apply femtosecond laser pulses to ZnSe bulk material to investigate exciton resonances. The non-linear technique of optical second harmonic generation (SHG) allows us to test other excitation rules than in linear optics. Despite the broad bandwidth of the laser pulses we succeed to measure narrow exciton resonances. We present measurements in different crystal directions without and in magnetic fields in voigt and faraday configuration. The polarisation dependency of the SHG intensity is analysed as well. Especially incident light in (100)-direction is of interest as the process of SHG is forbidden in this geometry in the electric-dipole approximation without magnetic field. The application of a magnetic field up to 10 T leads to a rich spectrum of exciton resonances which can be assigned to envelope-hole coupling of the 2P exciton and to landau-levels of the 2P and 3P exciton by comparison with calculations.

HL 27.11 Tue 12:30 H17

ODNMR studies of selenium nuclei in a flourine-doped ZnSe epilayer — •Erik Kirstein[1], Fabian Heisterkamp[1], Alexander Greilich[1], Evgeny A. Zhukov[1], Tomasz Kazimerczuk[1], Dmitri R. Yakovlev[1,2], Alexander Pawlis[3], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

A longitudinal (T_1) and transverse (T_2) relaxation times of selenium nuclei present in a fluorine-doped ZnSe epilayer are studied by optically detected nuclear magnetic resonance. Circularly polarized laser pulses optically orient the electron spins, which in its turn polarize the nuclei. The nuclear polarization of selenium reveals itself as an Overhauser field, affecting, in its turn, the electron Larmor frequency in tranverse magnetic field, measured by Kerr rotation [1]. The changes of the Larmor frequency are then analized in timescale to measure: the time needed for a complete polarization of the nulcear system under the optical excitation (T_{pol}), and the time needed for a system to come back to equilibrium in a complete darkness, T_1. Furthermore, radio frequency pulses are applied to measure the inhomogeneous T_2^* and homogeneous T_2 nuclear spin coherence using Ramsey and Hahn-Echo pulse sequences. Finally, we found that the spin temperature approach is fully justified for that system, as $T_1 \gg T_2$. [1] F. Heisterkamp, *et al.*, arXiv:1508.05295 [cond-mat.mes-hall]

HL 27.12 Tue 12:45 H17

Thermal annealing of GaAs nanowires studied by in-situ time-resolved x-ray diffraction — •Seyed M M Kashani[1], Philipp Schroth[1,2,3], Julian Jakob[2], Jonas Vogel[1], Martin Köhl[3], Tilo Baumbach[2,3,4], and Ullrich Pietsch[1] — [1]University of Siegen, Solid State Physics, Siegen, Germany — [2]Laboratory for Application of Synchrotron Radiation (LAS), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [3]Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [4]Synchrotron Facility ANKA, Karlsruhe Institute of Technology, Karlsruhe, Germany

In this contribution, we present a first attempt in studying the evolution of sublimation kinetics and polytypism during after-growth annealing of GaAs nanowires by in-situ X-ray diffraction and using a portable MBE chamber. The experiment has been performed at the beamline P09 of PETRA III (DESY) synchrotron using a wavelength of ~0.83 Å. Prior to annealing GaAs NWs were grown by self-catalyzed MBE onto Si(111). In a second step, the characteristic Bragg reflections of zinc-blende (ZB) (220) and (311), and wurtzite (WZ) (10.3) were simultaneously and repeatedly monitored during annealing at nine different temperatures ranging from 270°C to 670°C in steps of 50°C. The decomposition rate of ZB and WZ portions and NW diameters were determined from the evolution of integrated intensity and reflection shape, respectively. Whereas the intensity of WZ reflection decreases continuously, there is a discontinuity of ZB intensity at about 445+-25°C.