HL 87: ZnO: Growth and Defects

Time: Friday 10:15–13:30 Location: POT 51

HL 87.1 Fri 10:15 POT 51

Structural parameters of ZnMgO from first principles and experiment — •Marcel Giar[1], Thomas Wassner[2], Bernhard Laumer[1,2], Martin Eickhoff[1], and Christian Heiliger[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität, D-35392 Giessen, Germany — [2]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching, Germany

Recent experimental research on the variation of the lattice parameters of wurtzite ZnMgO with the Mg content x(Mg) show that the lattice parameter a strongly depends on the thickness of the prepared thin films. For layers with a thickness of about 300nm grown by molecular beam epitaxy a is found to be independent of x [1] whereas for thin films of 1μm we find an increase in a with increasing x. We conduct cell relaxations keeping the lattice parameter a fixed in the basal plane as well as complete cell relaxations using the LDA and a supercell approach to account for both effects known from experiment. We further employ alloy statistics to consider different alloy configurations inside the supercell. Theoretical and experimental results for the lattice constants a and c and related parameters are compared showing a good qualitative agreement.

[1] T. A. Wassner, B. Laumer, S. Maier, A. Laufer, B. K. Meyer, M. Stutzmann, M. Eickhoff, J. Appl. Phys. 105, 023505 (2009)

HL 87.2 Fri 10:30 POT 51

Defect Reduced Growth of Pulsed Laser Deposited ZnO — •Fabian Budack, Marc A. Gluba, Lars-Peter Scheller, and N.H. Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie, Kekuléstr. 5, 12489 Berlin, Germany

Zinc oxide is a transparent semiconductor with a pronounced doping asymmetry. While electron conduction is easily achieved even in nominally undoped material reliable and stable p-type doping was not yet realized. Beside hydrogen, intrinsic defects have been discussed as the origin of the prevailing n-type conduction. Understanding the conditions for the formation of native donor-like defects is a necessary step towards obtaining stable p-type ZnO.

Nominally undoped, albeit n-type, ZnO thin films have been deposited by pulsed laser ablation (PLD) on sapphire and MgO substrates under varying oxygen partial pressures. Both, structural parameters like growth rate as well as electrical properties, were investigated. It is found that the carrier concentration shows a distinct minimum at oxygen partial pressures of 5 to $7 \cdot 10^{-4}$ mbar while the mobility is nearly constant over a broad range of partial pressures. The decrease of the electron concentration is accompanied by an increasing growth rate, indicating a defect reduced growth mode in the presence of oxygen. However, a further increase of the deposition pressure leads to the formation of nanostructures, which results in new defects. This trade-off and its impact on the doping asymmetry of ZnO will be discussed.

HL 87.3 Fri 10:45 POT 51

Electrochemical deposition of ZnO for Flexible Electronic Devices — •Miriam Schwarz and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Electrochemical deposition from aqueous zinc nitrate ($Zn(NO_3)_2$) solution provides a simple way to deposit crystalline ZnO at low temperatures. Thus, it is a suitable process for flexible substrates like polyethylenterephthalat (PET) foil and makes ZnO to an interesting alternative in the field of flexible electronics in comparison to organic counterparts. The electrochemical approach allows to strongly influence the morphology of the ZnO layer by many well defined deposition parameters like the applied voltage, temperature, time and electrolyte concentration. This correlation is investigated by atomic force microscopy (AFM) and scanning electron microscopy (SEM) for the morphology of the ZnO layer, while Raman spectroscopy is applied to evaluate the crystalline quality of the layers. It reveals that ZnO crystallites of hexagonal shape with diameters depending on the deposition parameters are achieved. In order to study the correlation between the ZnO morphology and its electrical performance in devices, Schottky diodes and field-effect transistors were manufactured and systematically analyzed.

HL 87.4 Fri 11:00 POT 51

Incorporation of dopant atoms into zinc oxide surface layers using ultrashort laser pulses — •Andreas Schneider, Apurba Dev, Kathrin Sebald, and Tobias Voss — Institut für Festkörperphysik, Bremen, Germany

The exposure of semiconductors to ultrashort laser pulses can lead to ultrafast melting and ablation of their surfaces. These non equilibrium processes create quasi-periodic surface structures. For silicon, these micro-structured surfaces - often called black silicon - show a strong increase of the absorption above and below its bandgap in a sulphurous environment creating an extremely highly doped surface layer. We apply a similar approach for zinc oxide. A thin layer of antimony is vapor-deposited on a bulk c-plane wafer followed by structuring the sample with amplified 100fs laser pulses. After multiple pulses, the zinc oxide surface shows a ripple pattern. Steep trenches run down to 3μm into the bulk. Cross sectional TEM measurements reveal a 200nm thick polycrystalline layer on top of the ripple structure. Below this layer the ripples are single crystalline. EDX measurements show that antimony was incorporated to the first 260nm, resulting in the tracing of antimony even in the single crystalline region. The exact amount of incorporation and the surface morphology strongly depend on the applied structuring parameters. Using SEM we find that increasing the laser fluence also increases the observed ripple period. In contrast to this a larger number of pulses leads to smaller ripple periods as well as steeper and deeper trenches. Our results are a promising step towards doping zinc oxide surface layers by ultrashort laser pulses.

HL 87.5 Fri 11:15 POT 51

Dominant Laplace DLTS peaks E280 and E290 in melt-grown ZnO — •Leopold Scheffler, Vladimir Kolkovsky, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

In the present study single-crystal ZnO grown from the melt was investigated by electrical measurements such as DLTS and high-resolution Laplace DLTS. A peak E280 dominates the DLTS spectrum in the wide temperature range of 20-450 K. Using high-resolution Laplace DLTS this peak was found to consist of two levels with activation energies of 280 meV and 290 meV below the conduction band, respectively. The relative intensities of these peaks depend on the measurement temperature. The thermal stability of the defects in oxygen and oxygen-lean atmosphere is analyzed. The origin of these defects will be discussed.

HL 87.6 Fri 11:30 POT 51

Metastable state of the $V_{Zn}H_2$ defect in ZnO — •Dirk Bastin, Edward Lavrov, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

The Zn vacancy passivated by two hydrogen atoms in ZnO $V_{Zn}H_2$ was studied by IR absorption spectroscopy. It was shown that in addition to the ground state comprising two inequivalent O-H bonds aligned parallel and 'perpendicular' to the c-axis of the crystal, there is a metastable state of the defect ($V_{Zn}H_2^*$). $V_{Zn}H_2^*$ consists of two equivalent O-H bonds oriented 'perpendicular' to the c-axis. The metastable state of the Zn vacancy decorated with two hydrogen atoms reveals two local vibration modes at 3329.0 and 3348.4 cm^{-1} which represent antisymmetric and symmetric combinations of the two separate O-H stretch modes, respectively. The energy difference between the ground and the metastable states of the complex was found to be 75±9 meV. It was also established that the activation energy of the hydrogen motion within the Zn vacancy is 0.96±0.09 eV.

15 min. break

HL 87.7 Fri 12:00 POT 51

Ion-beam Induced Luminescence in n-type Zinc Oxide — •Ronald Stübner[1], Matthias Allardt[1], Daniel Severin[2], Markus Bender[2], and Jörg Weber[1] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

Ion implantation of semiconductors introduces a wide variety of defects. Their concentration and depth profile depends on the energy and the fluence of the ions as well as on the temperature of the sample during the irradiation. The in-situ monitoring of these defects helps to understand the creation mechanism and kinetics of the different

kinds of defects. The design and assembly of an ionoluminescence measurement system was done during a diploma thesis. The system has been installed at the M-Branch of the ion accelerator at the GSI Helmholtz Centre for Heavy Ion Research in Darmstadt where samples of n-type ZnO single crystals have been irradiated at room temperature and low temperatures, respectively. In this talk, the results of these measurements as well as the results of subsequent photoluminescence investigations will be presented.

HL 87.8 Fri 12:15 POT 51

$Zn_{1-x}Cd_xO$ thin films and heterostructures grown by pulsed laser deposition — •Martin Lange, Christof P. Dietrich, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Linnéstr. 5, D-04103 Leipzig, Germany

Effecient optoelectronic devices are based on heterostructures which require band gap engineering. A reduction of the ZnO bandgap is possible when Cd is incorporated.[1] Here, we present an ansatz allowing the incorporation of up to 24 % Cd in ZnO without a phase separation using pulsed laser deposition. Therefore, we applied low substrate temperatures down to room temperature. A red-shift of the near band-edge luminescence down to energies of approximately 2.6 eV was achieved.

We used mixed targets of ZnO and CdO and were therefore able to grow the $Zn_{1-x}Cd_xO$ directly on the *a*-plane saphire substrates without surrounding ZnO layers. The thin films exhibit a wurtzite crystal structure with the *c*-axis parallel to the growth direction. With increasing Cd-content the *c*-axis constant increases in agreement with literature.[2] The bandgap energy decreases with increasing Cd-content, which was verified by a red-shift of the luminescence maximum and the absorption edge of the $Zn_{1-x}Cd_xO$.

Finally, $Zn_{1-x}Cd_xO$ was combined with ZnO thin films and ZnO nanowires in various heterostructures.

[1] S. Sadofev *et al.*, Appl. Phys. Lett. **89**, 201907 (2006)
[2] K. Yamamoto *et al.*, J. Cryst. Growth **312**, 1703 (2010)

HL 87.9 Fri 12:30 POT 51

Strain-related defects in $Mg_xZn_{1-x}O$ thin films — •Florian Schmidt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

We investigated the influence of tensile and compressive strain, respectively, on the incorporation of deep levels defects in $Mg_xZn_{1-x}O$ thin films grown by pulsed-laser deposition on *a*-plane sapphire substrates. For ZnO it was recently shown that tensile strain induces a new defect level traceable via photoluminescence by the recombination line I_{12} [1]. In order to investigate thin films under tensile and compressive strain, respectively, we chose Al-doped ZnO as buffer layer, which has a larger *a*-lattice constant than that of ZnO and can be used as an ohmic back-contact due to its low resistivity. The *a*-lattice constant of $Mg_xZn_{1-x}O$ increases with x, so the Mg-content can be used to change the strain state of the thin film from tensile to compressive strain. Therefore, we changed the Mg-contents in the samples from $x = 0$ to 0.02. In concordance with ref. [1] we observe the I_{12} transition in low temperature photoluminescence measurements only if the samples are under tensile strain. Further we have found by deep level transient spectroscopy (DLTS) and Laplace DLTS that the two deep level defects, labelled T2 and E3' in the literature, are detectable only in thin films under tensile strain. The E3' defect level is most likely an extended defect formed to relief stress. Independent of the strain state the two defect levels E100 and E3 are detected.

[1] M. Brandt *et al.*, Phys. Rev. B **81**(7) 073306 (2010)

HL 87.10 Fri 12:45 POT 51

Strain distribution in ZnO microwires — •Christof P. Dietrich, Martin Lange, Fabian J. Klüpfel, Rüdiger Schmidt-Grund, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Abteilung Halbleiterphysik, Institut für ExperimentellePhysik II, 04103 Leipzig, Germany

We present a direct experiment to determine the strain dependence of semiconductor energy bands with high precision. For this purpose we benefit from the unique properties of self-organized grown ZnO microwires with respect to their excellent crystal quality and the possibility to easily adjust the strain in such objects by bending, opposite to thin films or bulk single crystals. In order to study the band gap energy variation with strain we measure the related photoluminescence (PL) of the exciton recombination spatially resolved at low temperatures on mechanically bent ZnO microwires fabricated by carbothermal reduction. We show that mechanical bending leads to a significant blue and red-shift of the wire luminescence due to the formation of compressive and tensile strained parts of the wire, respectively. Linescans perpendicular to the wire axis showed maximum energetic shifts of the dominant recombination peaks of ±30 meV due to strain values of ±1.5 %. The compressive and tensile strain inside the wires turned out to be symmetrically distributed perpendicular to the wire axis meaning that the neutral fibre coincides with the central wire axis. From these experiments, we are able to precisely determine the deformation parameter that connects the energetic shift of the wire luminescence and the applied uniaxial stress.

HL 87.11 Fri 13:00 POT 51

On the T2 deep level in zinc oxide thin films — •Matthias Schmidt[1,2], Robert Karsthof[1], Florian Schmidt[1], Holger von Wenckstern[1], Martin Ellguth[1], Rainer Pickenhain[1], Marius Grundmann[1], and Gerhard Brauer[2] — [1]Universtity of Leipzig, Institute for Experimental Physics II, Linnéstraße 5, D-04103 Leipzig — [2]Forschungszentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Postfach 51 01 19, D-01314 Dresden

For the majority of deep levels studied in n-type conducting ZnO by means of capacitance spectroscopy only the activation energy and the high temperature limit of the electron capture cross-section are known since these quantities can be evaluated easily from the temperature dependence of the trap's thermal electron emission rate.

We focused on the T2 level present in ZnO thin films grown by pulsed laser deposition. In order to tune the T2 concentration in the samples, we employed different growth and annealing conditions as well as the implantation of oxygen and zinc ions, respectively. The physical properties of T2 were studied by different deep level transient spectroscopy and photo- capacitance experiments. These experiments revealed a strong dependence of the thermal activation energy, 185meV<E<280meV, on the concentration of T2 in the sample as well as on the electric field (Poole-Frenkel effect). T2 was found to be preferentially generated under zinc rich conditions as both, the implantation of zinc ions and thermal annealing at low oxygen partial pressures increase its concentration. From photo- capacitance transients the photo- ionisation cross- section spectrum was calculated.

HL 87.12 Fri 13:15 POT 51

Low temperature CVD-synthesis of nitrogen doped ZnO thin films — •Sebastian Eisermann, Stefan Lautenschlaeger, Michael N. Hofmann, Andreas Laufer, Melanie Pinnisch, Christian Reindl, Julian Benz, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen

We report on the growth of nitrogen doped ZnO thin films prepared at low temperatures by chemical vapour deposition. As substrates, polar and non-polar ZnO single crystals were used. The successful incorporation of nitrogen into the ZnO matrix was confirmed by Secondary Ion Mass Spectrometry (SIMS) and Raman measurements. The optical features were examined by photoluminescence (PL) analysis. Furthermore, ZnO diode structures were fabricated and investigated by IV-measurements. The PL spectra of the nitrogen doped films show a pronounced Donor-Acceptor-Pair-Recombination (DAP) in the energy-region of 3.25 eV. The intensity of this luminescence feature increases with increasing nitrogen content. The IV-measurements reveal typical diode-like behaviour of the ZnO diode structures.