HL 32: Poster I: Group II - Oxides

Time: Tuesday 18:30–20:30 Location: Poster D1

HL 32.1 Tue 18:30 Poster D1

Parameter-free calculations of electronic properties and optical transitions of MgO, ZnO, and CdO — •André Schleife, Claudia Rödl, Frank Fuchs, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Jena, Germany

With the computational capabilities that are available nowadays it is possible to drive modern parameter-free calculations towards predictive accuracy. This development made *ab-initio* methods an inevitable tool for materials science when experimental access is impossible, e.g., for non-equilibrium crystal structures.

In our calculations for three important oxide materials we employ the nonlocal hybrid HSE03 functional as approximation to exchange and correlation, even including spin-orbit coupling. Quasiparticle energies are calculated by means of Hedin's *GW* approximation, involving screening of the electron-electron interaction from the fully frequency-dependent dielectric function.

This sophisticated approach is used to derive unknown quantities for MgO, CdO, and ZnO in the wurtzite structure: fundamental gaps, effective electron and hole masses, crystal-field and spin-orbit splittings, optical transition matrix elements, and even exciton binding energies. Chemical trends are pointed out.

HL 32.2 Tue 18:30 Poster D1

Oxygen vacancy and nitrogen substitutional in ZnO: An ab initio study — •Fabian Hachenberg, André Schleife, Jürgen Furthmüller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

In the last decade, the wide-gap semiconductor ZnO has attracted large attention due to its potential use in optoelectronic applications. Still the difficulty of reliable and reproducible p-type doping is an obstacle in using ZnO for light-emitting devices. Therefore, a comprehensive understanding of the behaviour of point defects in ZnO is crucial. We present first-principles calculations for the electronic and structural properties of two important point defects in different charge states in ZnO. Using a supercell approach we study the oxygen vacancy and the nitrogen substitutional. The calculations are carried out using generalized-gradient corrected density functional theory (DFT-GGA) and pseudopotentials within the projector-augmented wave (PAW) framework. For studying the electronic structure we also employ the GGA+U method and the nonlocal HSE03 exchange and correlation functional. We discuss errors induced by the semilocal GGA, as well as supercell-specific finite-size effects. We derive formation energies and transition levels for both point defects and compare to other calculations and also experimental results.

HL 32.3 Tue 18:30 Poster D1

First principles calculation of inter- and intra-band Auger recombination rates in ZnMgO — •Markus Heinemann and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392 Giessen, Germany

Recent theoretical work on GaInN [1] indicates that inter-band Auger recombination causes a resonance in the Auger coefficient in the blue to green spectrum which leads to a loss in quantum efficiency of nitrite based light emitters. We report ab initio investigations on non-radiative loss mechanisms due to band-to-band Auger recombination in wurtzite ZnMgO alloys. We use density functional theory to compute inter- and intra-band Auger recombination rates as a function of the Mg concentration.

[1] K. T. Delaney, P. Rinke, and C. G. Van de Walle, Appl. Phys. Lett. 94, 191109 (2009)

HL 32.4 Tue 18:30 Poster D1

Ab initio studies on the structural parameters of ZnMgO alloys — •Marcel Giar, Markus Heinemann, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, 35392 Giessen, Germany

Experimental and theoretical investigations on the lattice parameters of $Zn_{1-x}Mg_xO$ alloys in wurtzite structure show a decreasing c-axis and an increasing a-axis with increasing Mg concentration [1,2]. The *ab initio* computations [2] are based on density functional theory (DFT) in the local density approximation (LDA). We perform first-principle DFT calculations using the LDA as well as the generalized gradient approximation (GGA) for the exchange correlation functional. We determine the equilibrium lattice parameters of wurtzite $Zn_{1-x}Mg_xO$ alloys for different compositions ranging from $0 \leq x \leq 31.25$ %. For the lattice constants a and c we find the same qualitative behavior as reported in [1] and [2]. LDA results show the typical underestimate of the lattice parameters while the values obtained by GGA excess the experimental results. We further find a deviation from Vegard's law. For the unit cell volume we see a constant behavior independent of the Mg concentration.

[1] A.Ohtomo and A. Tsukazaki, *Semicond. Sci. Technol.* **20**, S1-S12 (2005)
[2] X. F. Fan, H. D. Sun, Z. X. Shen, Jer-Lai Kuo and Y. M. Lu, *J. Phys. Cond. Mat.* **20** 235521 (2008)

HL 32.5 Tue 18:30 Poster D1

Capacsim - numerical modelling of the capacitance of a current-free Schottky diode — •Matthias Schmidt, Martin Ellguth, Holger v. Wenckstern, Rainer Pickenhain, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Schottky diodes (SD) are under investigation for more than 50 years and are a powerful tool in semiconductor defects research. A number of different techniques, each of them somehow connected to the capacitance, or more generally the admittance, were established: e.g. capacitance - voltage spectroscopy (CV), thermal admittance spectroscopy (TAS), and photo capacitance (PCAP).

We developed a numerical model to calculate the admittance of a SD. It provides a realistic reproduction of the influence of six independent parameters - the applied bias, the probing voltage and frequency of the capacitance bridge, the temperature, and illumination of the sample, parameterised by the photon flux and the photon energy. The model takes into account the potential distribution at the Schottky barrier which is calculated numerically in the general case. In case of homogeneous doping of the sample, an analytical solution is used. Furthermore, the time evolution of the occupancy of a trap surrounded by an oscillating electron environment is considered and provides information on the contribution of the local trap density to the measured admittance.

Finally exemplary simulations and a comparison with CV, TAS, and PCAP measurements on real zinc oxide Schottky diodes are presented.

HL 32.6 Tue 18:30 Poster D1

Spin Noise Spectroscopy of ZnO — •Hauke Horn[1], Xavier Marie[2], Andrea Balocchi[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Gottfried Wilhelm Leibniz University Hannover, Appelstr. 2, 30167 Hannover, Germany — [2]INSA-CNRS-UPS, LPCNO, Université de Toulouse, 135 Av. de Rangueil, 31077 Toulouse, France

ZnO is a promising material for optical spintronics showing long electron spin lifetimes due to the large band gap and low amount of nuclear spin isotopes. Here, we use spin noise spectroscopy to access the electron spin dynamics of this material in thermal equilibrium while avoiding carrier heating and excitation of electron hole pairs.

A linear polarized laser beam ($E_{\mathrm{UV-Laser}} = 3.32$ eV) close to the direct band gap of ZnO ($E_{D^0X} = 3.36$ eV) is used to detect the spin dynamics of neutral donors in ZnO with off–resonant, non–demolition Faraday rotation. The stochastic oriented electron spins induce polarization fluctuations of the transmitted laser beam. The fluctuation strength of N non–interacting, paramagnetic spins follow the Poisson statistics and generate measurable noise $\propto \sqrt{N}$ spins. These fluctuations are measured via a polarization bridge in the radio frequency regime and Fourier transformed in real–time. A magnetic field B is applied in Voigt–geometry and modulates the noise signal with the Larmor frequency of the electron spins $\omega_L = g\mu_B B/\hbar$. From the recorded noise spectra we can extract the electron g–factor, spin lifetimes, and densities.

HL 32.7 Tue 18:30 Poster D1

Investigation of piezoelectric and thermoelectric properties of ZnO microstructures — •Irina Laubenstein[1], Marcel Ruth[1], Alexander M. Bernhart[2], Johannes Schaffert[2], Christian A. Bobisch[2], Rolf Möller[2], and Cedrik Meier[1] — [1]University of

Paderborn, Experimental Physics & CeOPP - Center for Optoelectronics & Photonics Paderborn, Warburger Str. 100, 33098 Paderborn — [2]University of Duisburg-Essen, Experimental Physics, Lotharstr. 1, 47057 Duisburg

Metal oxides are highly attractive in high-temperature thermoelectric applications due to their inherent oxidation resilience and thermal resistance. Especially zinc oxide (ZnO) is a promising candidate. Alloying can increase the electric conductivity and at the same time decrease the thermal conductivity. Going to nanoscale dimensions, even less thermal conductivity is expected, because of phonon barriers caused by additional interfaces.
We demonstrate the first results of Seebeck-coefficient measurements on especially developed ZnO-microstructures as an intermediate step towards ZnO-nanostructures. Commercially available hydrothermally grown ZnO-crystals as well as plasma-assisted MBE (molecular beam epitaxy) grown ZnO-epilayers on c-plane sapphire substrates are used as basis materials. Furthermore, we investigate the piezoelectric properties of the devices by controllably exerting an external force using a UHV-four-probe scanning tunneling microscope (STM).
Financial support by BMBF via the NanoFutur grant 03X5509-NanoPhox & DFG via SFB616.

HL 32.8 Tue 18:30 Poster D1

Transport properties of ZnO along a- and c-crystallographic directions — •Christian H. Will, Matthias T. Elm, Sebastian Eisermann, Stefan Lautenschläger, Bruno K. Meyer, and Peter J. Klar — 1. Physikalisches Institut, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen

ZnO layers were grown on r-plane and c-plane sapphire substrates by chemical vapor deposition (CVD) resulting in c- and a-plane orientated ZnO layers, respectively. In order to investigate the transport properties along the different crystal directions, the samples were Hall-bar-structured by photolithography, followed by a wet chemical etching step in a solution of water (H_2O), phosphoric acid (H_3PO_4) and acetic acid ($C_2H_4O_2$) in parts of 30:1:1 by volume. On the a-plane ZnO, the Hall-bars were orientated such that the current could be applied either parallel to the a- or parallel to the c-direction of the crystal. For c-plane ZnO, the current direction is along the crystallographic a-direction. Magneto-transport measurements were performed in the temperature range from 1.6 to 280 K in external magnetic fields up to 10 T in order to determine the magnetoresistance, the Hall constant and the mobility as functions of temperature. The resulting transport properties for the different Hall-bar orientations will be compared and analyzed.

HL 32.9 Tue 18:30 Poster D1

Investigations on the stability of zinc oxide based metal-semiconductor field-effect transistors — •Michael Lorenz, Heiko Frenzel, Alexander Lajn, Holger von Wenckstern, Holger Hochmuth, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

Metal-semiconductor field-effect transistors (MESFETs) were fabricated by reactive dc-sputtering of Ag, Pd and Pt as Schottky-gate contact on ZnO thin films grown by pulsed-laser deposition and by rf magnetron sputtering on glass substrates. With on/off-current ratios of up to 10^6 and channel mobilities at around 1 cm^2/Vs [1] the devices are a potential alternative to currently used a-Si based switching thin film transistors (TFTs) in display applications. For a reasonable operation the MESFETs have to be resistent against light illumination, raised temperatures and require a long lifetime under bias stress without the degradation of their field-effect properties. We present studies of the influence of light with different wavelenghts as well as effects of temperatures in the range of 25°C and 150°C on the electrical properties of the MESFETs. Beside the influence of time the bias stress stability and different gate geometries on the field-effect charactersitics of the TFTs are shown.
[1] H. Frenzel *et al.*, Appl. Phys. Lett. **95**, 153503 (2009)

HL 32.10 Tue 18:30 Poster D1

Space-charge regions in ZnO-based metal-semiconductor field-effect transistors and metal-semiconductor-metal photodetectors — •Zhipeng Zhang, Michael Lorenz, Lucie Behnke, Christian Czekalla, Heiko Frenzel, Gisela Biehne, Holger Hochmuth, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstraße 5, 04103, Leipzig

We present current-voltage and light beam induced current (LBIC) investigations of metal-semiconductor field-effect transistors (MESFETs) and interdigital metal-semiconductor-metal photodetectors (MSM-PDs). The Schottky-contacts were fabricated by reactive DC-sputtering of palladium (Pd) with a Pd-capping [1] on nominally undoped ZnO thin films, heteroepitaxially grown by pulsed-laser deposition on sapphire and quartz glass [2]. They exhibit ideality factors < 1.5 and effective barrier heights > 0.8 V. The normally-on PdO_x-gate MESFETs have an on/off-ratio of 10^3 and channel mobilities of $0.3\,cm^2/Vs$. The LBIC measurements enable us to probe the lateral extension of the space-charge regions and homogeneity of the carrier distribution in the samples.
[1]: A. Lajn *et. al.*, J. Vac. Sci. Technol. B, **27**, 1769 (2009)
[2]: H. Frenzel *et. al.*, Appl. Phys. Lett., **95**, 153503 (2009)

HL 32.11 Tue 18:30 Poster D1

Growth and doping of ZnO nanorods — •Cornelius Thiele, Janos Sartor, Felix Eilers, Jonas Conradt, Claus Klingshirn, and Heinz Kalt — Institut für Angewandte Physik, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

The growth of ZnO nanorods has attracted a large interest in recent years, due to the abundance of the material and the relative ease of manufacturing such structures. The controllable doping of these structures is in the focus of our work, because almost all applications would benefit from a controllable conductivity. In our case the particular interest is to increase the electron transport in P3HT:PCBM hybrid solar cells by integrating ZnO nanorods. We grow nanorods on different substrates in a vapor phase transport process under high (950°C) and low (500°C) temperatures and investigate different methods of dopant integration. We examine in-situ doping during growth as well as evaporation and in-diffusion of donator materials afterwards. The effects of annealing time, temperature and atmosphere on the donor diffusion are studied by low-temperature photoluminescence measurements.

HL 32.12 Tue 18:30 Poster D1

ZnO-based Nanowire Structures and Heterostructures — •Martin Lange, Christof Peter Dietrich, Christian Czekalla, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, D-04103 Leipzig, Germany

Nanowires are ideal building blocks for future optoelectronic applications. For the fabrication of devices based on heterostructures, bandgap engineering is required, alloying ZnO e.g. with Mg and Cd. The alloys of ZnO with Mg results in a larger bandgap whereas it is reduced for Cd. The growth of alloy nanostructures is often much more challenging than the growth of the alloy thin films as the freedom in the choice of the growth parameters is reduced.

We report on the growth and optical properties of ZnO-based nanowire structures and heterostructures grown by pulsed laser deposition. A ZnO layer on *a*-sapphire was used as substrate to grow the nanowires in the regime of low density, allowing a more controlled growth mode and easier access to single nanowires than for high densities. For the implementation of quantum wells into the heterostructures, a core with a large bandgap is reasonable. In this context, MgZnO-nanowires were investigated. For the quantum well itself ZnCdO is a promising material. Therefore (Mg)ZnO nanowires were coated with a ZnCdO shell and an outer (Mg)ZnO shell forming a nanowire core-shell-structure.

HL 32.13 Tue 18:30 Poster D1

Growth and characterization of ZnO- and ZnO:P-microwires — •Christof P. Dietrich, Martin Lange, Jan Zippel, Jörg Lenzner, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

Currently, there is an extreme interest in fabricating small sized ultraviolet emitting devices such as LEDs or lasers. The wurtzite semiconductor ZnO is a promising candidate for such applications due to its band gap at 3.4 eV and its large exciton binding energy allowing the observation of excitonic recombination at room temperature and above.

ZnO is a native *n*-type semiconductor. Stable *p*-type conductivity can be achieved by the incorporation of phosphorus atoms into ZnO [1]. Micrometer sized ZnO- and ZnO:P-rods were grown by a thermal reduction process using carbon as reductant.

We give detailed insight into the growth process of ZnO-based microstructures and their morphology. Furthermore, we present a comprehensive study of the optical and electrical properties of ZnO- and ZnO:P-microwires using cathodoluminescence spectroscopy and Hall effect measurements, respectively.

[1] B.Q. Cao et al., phys. stat. sol. (RRL) **2**, 37-39 (2008).

HL 32.14 Tue 18:30 Poster D1

Implantationsuntersuchungen von ^{100}Pd in ZnO und GaN — •Patrick Kessler[1], Heiko Timmers[2], Aidan P. Byrne[3], Mark Ridgway[4] und Reiner Vianden[1] — [1]Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn — [2]School of Physical, Environmental and Mathematical Sciences, University of New South Wales at the Defence Force Academy, Canberra — [3]Department of Nuclear Physics and Department of Quantum Science, Research School of Physics and Engineering, Australian National University, Canberra — [4]Electronic Materials Engineering, Australian National University, Canberra

Durch eine Dotierung mit Übergangsmetallen (ÜM) wie Co, Mn oder Fe ist nach Dietl et al [1] Ferromagnetismus von ZnO und GaN bei Raumtemperatur möglich. Mit der Sonde ^{100}Pd, die isoelektronisch zu Co ist, wurde mit der Methode der gestörten Winkelkorrelation (PAC) ZnO und GaN untersucht. Durch das große magnetische Moment der Sonde ist man sehr empfindlich auf interne Magnetfelder am Ort des ÜM.

^{100}Pd wurde am 14UD Pelletron der ANU in Canberra Rückstoßimplantiert. Um das Ausheilverhalten zu studieren wurde ein isochrones Anlassprogramm durchgeführt. Dabei zeigen die untersuchten Halbleiter keinen substitutionellen Einbau der Sonden, obwohl dies mit anderen implantierten Sonden problemlos möglich ist (In, Br, Cd). RBS-Channelling-Messungen an stabilem Pd deuten auf Clusterbildung des ÜM hin.

[1] T. Dietl, Science, vol. 287, pp. 1019-1022 (2000)

HL 32.15 Tue 18:30 Poster D1

Sputter deposited gallium doped ZnO for TCO applications — •Marc Dietrich[1], Achim Kronenberger[1], Angelika Polity[1], Bruno Meyer[1], Jürgen Bläsing[2], and Alois Krost[2] — [1]I. Physikalisches Institut, Justus Liebig Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]FNW/IEP/AHE, Otto-von-Guericke Universität Magdeburg, Postfach 4120, 39016 Magdeburg, Germany

Transparent conducting oxides to be used for flat panel or display applications should exhibit low electrical resistivity in line with a high optical transmission in the visible spectral range. Today indium-tin-oxide is the material which meets these requirements best. However, the limited availability of indium makes it useful to search for alternatives and ZnO doped with group III elements are promising candidates. While the Al doping in high concentrations causes problems due to the formation of insulating Al-oxides, Gallium related oxides are typically n-type conducting wide band gap semiconductors. Therefore we deposited Gallium doped ZnO thin films on quartz and sapphire substrates by radio frequency magnetron sputtering with a ZnO/Ga_2O_3(3at%) composite target. The substrate temperature and the oxygen flow during the sputtering process were varied to optimise the layer properties. Introducing oxygen to the sputtering gas allowed to vary the resistivity of the films by three orders of magnitude from about 1 Ωcm down to less than 1 mΩcm.

HL 32.16 Tue 18:30 Poster D1

Properties of hydrogen doped ZnO films prepared by RF magnetron sputtering — •Achim Kronenberger, Marc Kostantin Dietrich, Steve Petznick, Daniel Horn, Andreas Laufer, Jan Eric Stehr, Angelika Polity, Detlev Michael Hofmann, and Bruno Karl Meyer — I. Physics Institute, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

It is well known that hydrogen incorporated into ZnO induces shallow donor levels while in most other semiconductors hydrogen counteracts the prevailing conductivity by being incorporated as H+ (a donor) in p-type and as H- (an acceptor) in n-type material. Therefore, besides the Group III elements Al, Ga and In, hydrogen is suitable to control n-type conductivity in ZnO.

In our work hydrogen doped ZnO thin films were prepared by reactive radio frequency magnetron sputtering using a ceramic ZnO target. In the deposition process argon was used as sputtering gas and hydrogen and oxygen as reactive gases.

The structural (XRD), electrical (Hall-effect) and optical (Transmission) film properties were analyzed. Secondary ion mass spectrometry (SIMS) was used to quantify the hydrogen incorporation and electron spin resonance (ESR) measurements were used to detect the nature of the shallow donor. The thermal stability of hydrogen in the ZnO layers was examined by annealing experiments. Also long-term stability was investigated.

By varying the deposition parameters we were able to adjust the carrier concentrations from 10^{13} cm^{-3} up to the 10^{20}.

HL 32.17 Tue 18:30 Poster D1

Influence of ion-beam etching on the transport properties and the structural quality of microstructured zinc-oxide layers — •Markus Piechotka, Martin Fischer, Torsten Henning, Bruno K. Meyer, and Peter J. Klar — 1. Physikalisches Institut, Justus-Liebig-Universität, 35392, Gießen

We developed a wire pattern which is defined on zinc-oxide layers using photolithography and transfered into the layer using ion-beam etching. We investigated the transport behavior and the structural quality of the wire samples obtained. Ion-beam etching is a promising alternative to wet-chemical etching as higher aspect ratios may be achieved. A possible disadvantage is the structural damage of the layer due to ion implantation (gas or mask ions) as well as due to ion scattering processes deep inside the layer or substrate.

The structured samples were investigated by Raman microscopy in back scattering geometry using a 633 nm, 532 nm and 325 nm laser excitation, respectively. This yields information about vibrational modes and possible lattice defects such as impurities or vacancies. In addition the surfaces of the samples were studied via AFM and SEM in order to examine the structural quality and to determine the geometric dimensions of the individual wires. Furthermore we performed magnetotransport measurements to study the electronic transport properties after the etching treatment, mainly to investigate the influence of the damaged region on the electronic properties.

HL 32.18 Tue 18:30 Poster D1

Nitrogen Doping of Homoepitaxial a-plane ZnO — •Sebastian Eisermann, Stefan Lautenschlaeger, Michael Hofmann, Melanie Pinnisch, Andreas Laufer, Peter Jens Klar, and Bruno Karl Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen

Reproducible p-type doping of ZnO by nitrogen remains a challenge and evidence is found that the nitrogen incorporation depends on the growth plane during epitaxial growth. Thus we investigated the growth of nitrogen doped non-polar ZnO on a-plane ZnO-single-crystals using a metallic precursor CVD process. The nitrogen incorporation into the thin films has been analyzed by secondary ion mass spectrometry (SIMS) and the N-related vibrational modes were observed in Raman spectroscopy. Optical features of the layers such as the donor- and acceptor-bound-excitons have been investigated using low temperature photoluminescence (PL) measurements. The nitrogen incorporation in the non-polar films is possible while the incorporation of other impurities, especially group III impurities, seems to be diminished. This leads to a lower residual n-type conductivity.

HL 32.19 Tue 18:30 Poster D1

Nitrogen incorporation in ZnO thin films grown by chemical vapour deposition (CVD) — •Michael N. Hofmann, Stefan Lautenschlaeger, Sebastian Eisermann, Udo Roemer, Melanie Pinnisch, Andreas Laufer, Swen Graubner, Peter J. Klar, and Bruno K. Meyer — 1. Physics Institute, Justus-Liebig-University, Heinrich Buff Ring 16, 35392 Giessen, Germany

We determined the effect of different growth temperatures on the amount of nitrogen incorporation in thin ZnO films grown by chemical vapour deposition in a vertical growth configuration. Ammonia was chosen as nitrogen percurser, while ZnO a-plane and c-plane bulk crystals served as substrates. The grown films were investigated by Raman spectroscopy, photoluminescence and secondary ion mass spectroscopy. It turned out that low growth temperatures promote the incorporation of nitrogen. In contrast high growth temperatures are indispensable for achieving good crystal quality. We will show how to combine high nitrogen amounts with high crystal quality by in situ modulation of growth temperature and ammonia flux. Furthermore we investigated the influence of an additional annealing step on the samples.

HL 32.20 Tue 18:30 Poster D1

Electrical characterization of defects in MgZnO thin films grown by pulsed-laser deposition — •Kerstin Brachwitz, Hol-

ger von Wenckstern, Matthias Schmidt, Christof P. Dietrich, Marko Stölzel, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

We present electrical investigations on $Mg_xZn_{1-x}O$ semiconductor alloys, grown by pulsed-laser deposition. The Mg-content in the samples ranged from 0% to 40%. We investigated the structural and electrical properties of the thin films in dependence on the Mg-content. Furthermore we monitored changes of the activation energy of defect states after annealing for 30 minutes at different temperatures (500°C, 700°C and 900°C) in 700 mbar oxygen. High quality Schottky contacts were realized by reactive dc-sputtering of Pd. These Schottky diodes were used to investigate shallow and deep defect states using depletion layer spectroscopy. The thermal activation energy and the capture cross-section of the E3 defect have been determined in dependence on the Mg-content [1]. Shallow defects, already known in ZnO [2] were also observed in MgZnO and correlated with near band edge recombination spectra.

[1] H. von Wenckstern *et al.*, J. Electron. Mater., DOI: 10.1007/s11664-009-0967-0 (2009)

[2] F. D. Auret *et al.*, J. Phys. Conf. Ser. **100**, 042038 (2008)

HL 32.21 Tue 18:30 Poster D1

Laplace-transform deep-level transient spectroscopy in ZnO thin films — •Florian Schmidt, Holger von Wenckstern, Matthias Schmidt, Martin Ellguth, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

Deep-level transient spectroscopy (DLTS) is a space charge spectroscopic method commonly used for the characterization of semiconducting materials. The time constant resolution of standard DLTS using boxcar or lock-in techniques is however too poor for studying fine structure in emission processes. Digital transient processing, e.g. used in Laplace-transform deep-level transient spectroscopy (LDLTS), enables more sensitive deconvolution of capacitance transients.

We investigated ZnO thin films grown by pulsed-laser deposition by using LDLTS and demonstrated, that DLTS is not suited to characterize the two closely lying levels E3/E3' [1] appropriately. Instead, LDLTS is necessary to determine defect parameters as thermal activation energy E_t and apparent capture cross-section σ unambiguously. We found for E3 $E_t = 295\,\mathrm{meV}$ and $\sigma = 4 \times 10^{-16}\,\mathrm{cm}^2$ and for E3' $E_t = 386\,\mathrm{meV}$ and $\sigma = 4 \times 10^{-14}\,\mathrm{cm}^2$.

[1] F.D. Auret et al., Physica **B** 401-402 (2007) 378

HL 32.22 Tue 18:30 Poster D1

Defekt-Komplexbildung nach Ionenimplantation in ZnO — •Valentin Germic, Patrick Kessler und Reiner Vianden — Helmholtz Institut für Strahlen und Kernphysik, Universität Bonn

Nach der Implantation der Winkelkorrelationssonden ^{111}In oder ^{117}Cd und einer Anlasstemperatur von 900 K tritt ein Defekt auf, der allerdings bei höheren Temperaturen wieder ausheilt. Ein ähnlicher Defekt wurde bereits bei Winkelkorrelationsmessungen (PAC) von ^{111}In in ZnO nach der Dotierung mit Zn beobachtet [1]. Beides deutet auf eine mögliche Sauerstoffleerstelle hin. Dies könnte Hinweise für einen möglichen Mechanismus von Ferromagnetismus in Halbleitern geben, der durch die Bildung von magnetischen Polaronen aus Übergangsmetall-Ionen und einer Sauerstoffleerstelle entstehen [2].

Es kann gezeigt werden, dass die Defektbildung abhängig vom Implantationswinkel und unabhängig von der Ausheilatmosphäre ist. Durch eine PAC Orientierungsmessung wurden mögliche Positionen der Leerstelle im Kristallgitter bestimmt. Mit β-γ Korrelationsmessungen der Sonde ^{111}Ag ist abschließend die Bestimmung des Defekt-EFG Vorzeichens möglich.

[1] D. Forkel et al Mat. Res. Soc. Symp. Proc. 46 (1985) [2] J. M. D. Coey, Nature Materials 4, 173 - 179 (2005)

HL 32.23 Tue 18:30 Poster D1

Optical properties of transition metal doped ZnO — •Stephanie Jankowski[1], Limei Chen[1], Jonatan Helzel[1], Shuangli Ye[2], Carsten Ronning[3], Detlev Schulz[4], Birk Heimbrodt[4], Detlef Klimm[4], and Wolfram Heimbrodt[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, D-35032, Germany — [2]Institute of Microelectronics and Information Technology, Wuhan University, Wuhan 430072, China — [3]Physikalisch-Astronomische Fakultät, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena — [4]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 D-12489 Berlin, Germany

Various optical spectroscopy techniques have been used to investigate Co and Mn doped ZnO. Two series of samples were prepared for both (Zn,Co)O and (Zn,Mn)O. One series of ZnCoO thin films was grown by UHV-magnetron reactive sputtering and the other consists of ion implanted ZnO wires on a silicon substrate. The Mn doped series were fabricated by diffusion or by ion implantation of Mn in ZnO bulk material. The Mn and Co doped samples exhibit distinct differences in optical properties. In the case of the (Zn,Co)O the intern 3d transitions can be seen in PL as well as in absorption spectra. A broad Mn induced band is observable below the band gap in the absorption of the Mn doped samples. Details will be discussed at the poster.

HL 32.24 Tue 18:30 Poster D1

Photocurrent measurements of *a*- and *c*-plane oriented ZnO layers — •Richard K. Thöt, Thomas Sander, Sebastian Eisermann, Stefan Lautenschläger, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

We present in-plane photocurrent measurements of CVD-grown ZnO layers on different substrates. The measurements were performed at temperatures in the range from 80 K to 300 K. The spectra yield information about the influence of strain and crystal orientation on the interband transitions. At liquid nitrogen temperature a finestructure of the photocurrent response is visible due to transitions from multiple valence band energies. In another experiment we recorded photocurrent spectra using linearly polarized probe light varying the polarization angle. For *a*-plane grown ZnO samples the photocurrent confirms the expected anisotropy of the semiconductor layers. The finestructure of the valence band can be studied and the orientation of the *c*-axis within the layer can be determined.

HL 32.25 Tue 18:30 Poster D1

The refractive index of zinc oxide microwire single crystals — Christian Czekalla, Philipp Kühne, Chris Sturm, •Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstr. 5, 04103, Leipzig, Germany

Among a large number of applications, zinc oxide (ZnO) single crystals (bulk and micro- and nanowires) are expected to form important building blocks for future optoelectronic devices like light emitting and laser diodes. Optical resonances from ZnO structures have been observed by a number of groups in the past years.

In most of the publications, modeling of the mode structure, especially in the near bandgap spectral region, is difficult because the energy dependent refractive index $n(E)$ is typically not known. Additionally, in case of the self assembled micro- and nanowires, the structures are too small to perform spectroscopic ellipsometry to determine $n(E)$.

We compare $n(E)$ obtained from (a) spectroscopic ellipsometry measurements of ZnO bulk single crystals and (b) spatially resolved photoluminescence measurements of ZnO microwires employing a plane wave whispering gallery mode model for the observed resonances. We discuss the differences between the results obtained from the two methods and their mutual impact, leading to a highly precise determination of $n(E)$ in an energy range between 1.80 eV and 3.25 eV and for temperatures between 10 K and 295 K.

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Photolumineszenz- und Transmissionsmessungen an ZnO/MgZnO-Quantengrabenstrukturen — •Johannes Kupper, Alexander Müller, Gabriele Benndorf, Martin Lange, Matthias Brandt, Michael Lorenz und Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnestr. 5, 04103 Leipzig

Eine Möglichkeit zur Einstellung der Emissionswellenlänge von optischen Bauelementen bieten Quantengrabenstrukturen. Die Confinementenergie lässt sich über die Barrierenhöhe und Grabenbreite einstellen. Für Gräben aus ZnO eignet sich MgZnO als Barrierenmaterial. Mittels gepulster Laserabscheidung wurden einzelne ZnO/MgZnO-Quantengräben (QWs) mit unterschiedlicher Grabenbreite bei verschiedenen Züchtungsbedingungen auf *a*-Saphir abgeschieden. Dabei war es möglich QWs mit und ohne quantenunterstütztem Stark-Effekt (QCSE) darzustellen. Zur besseren Gitteranpassung wurde zwischen Grabenstruktur und Substrat eine MgZnO-Pufferschicht eingebracht.

Die QWs wurden mit Hilfe von Photolumineszenz(PL)- und Transmissions(TM)-Messungen zwischen 2K und 300K untersucht. Neben dem intensiven Hauptpeak der QW-PL zeigen sich mehrere Pho-

nonenwiederholungen, wobei die QWs mit QCSE eine zusätzliche Rotverschiebung der PL aufweisen. Die Grabenabsorption zeigt bis zu zwei Maxima. Das niederenergetische Maximum kann dem e1-h1-Übergang zugeschrieben werden. Die Zuordnung des höherenergetischen Maximums wird diskutiert.