HL 26 II-VI semiconductors II

Time: Tuesday 15:15–18:45 Room: POT 51

HL 26.1 Tue 15:15 POT 51

Homoepitaxial Growth of ZnO — •Stefan Lautenschläger, Arndt Zeuner, Joachim Sann, Niklas Volbers, Swen Graubner, and Bruno K. Meyer — I. Physikalisches Institut, Justus Liebig Universität Giessen, Heinrich Buff Ring 16, 35392 Giessen

ZnO, 1960's promising semiconductor, is regaining increased interest after the first reports of p-type doping. Its direct bandgap and total transparency for visible light suppose this material is suitable for many applications. Nowadays ZnO single crystals are available in sizes up to two inches.

Here we report on homoepitaxial growth of ZnO on ZnO single crystals with a home-bulit CVD epitaxy system. We were able to grow nominally undoped thin films of high quality. In doped samples we found the incorporation of nitrogen acceptors and lithium into the ZnO lattice.

All films were characterised by PL, XRD, SEM, SIMS and Hall measurements.

HL 26.2 Tue 15:30 POT 51

Defect mediated ferromagnetism in $Zn_{0.95}Co_{0.5}O$:(Cu,Al) thin films — •Lars Hartmann, Qingyu Xu, Heidemarie Schmidt, Holger Hochmuth, Michael Lorenz, Rüdiger Schmidt-Grund, Daniel Spemann, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstrasse 5, D-04103 Leipzig, Germany

Only recently it has been experimentally shown that defects mediate the ferromagnetism in $Zn_{0.95}Co_{0.05}O$ codoped Cu [1]. Cu is an acceptor lying only 0.17 eV below the ZnO conduction band [2]. Our work focusses on the optimization of defect mediated ferromagnetism in n-conducting $Zn_{0.95}Co_{0.05}O$:(Cu,Al) thin films grown by pulsed laser deposition on sapphire substrates. Numerical simulations [3] revealed that for codoping with $10^{20}cm^{-3}$ Cu and $10^{20}cm^{-3}$Al even at room temperature the Cu acceptors are occupied by unpaired electrons. The influence of the Co transition metal on the position of the Fermi level has been accounted for by growing ZnO:(Cu,Al) reference samples. By relating the temperature dependent position of the Fermi level with the experimentally determined free charge carrier concentrations, it will be shown how unpaired electrons being localized on the Cu acceptors influence the magnetoresistance of $Zn_{0.95}Co_{0.05}O$:(Cu,Al) thin films.

[1] M.H.F. Sluiter, Phys. Rev. Lett. 94 (2005) 187204
[2] Y. Kani, Jpn. J. Appl. Phys. 30 (1991) 703
[3] using NextNano3 (http://www.nextnano.de/)

HL 26.3 Tue 15:45 POT 51

Alloy Fluctuations and Phase separation in ZnCdO Layers: Thermalization and Carrier Freeze Out — •Alexander Franke[1], Thomas Hempel[1], Silke Petzold[1], Frank Bertram[1], Jürgen Christen[1], R. Kling[2], Christoph Kirchner[2], and Andreas Waag[3] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Department of Semiconductor Physics, Ulm University, Germany — [3]Department of Semiconductor Technology, Braunschweig Technical University, Germany

An inherent problem for the epitaxial growth ZnCdO is a different crystallization of ZnO and CdO into wurtzite and rock-salt structure, respectively resulting in local stoichiometry fluctuation and decomposition up to phase separation. A series of MOCVD grown $Zn_{1-x}Cd_xO$ layers with systematically increasing Cd-content (0.3%–2.0%) were analyzed using photoluminescence spectroscopy (PL). A systematic red-shift (3.239eV–3.150eV) and broadening of the PL peak is observed with increasing [Cd] merging into a splitting into two well distinguished peaks. While the high energetic main PL peak (dominant Cd-concentration) shows a linear excitation density dependence over more than 4 orders of magnitude, a super-linear dependence is found for the evolving satellite peak (minor Cd-rich local phase). The temperature dependence exhibits a pronounced s-shape behavior of the peak energy characteristic for thermalization and freeze out of the carriers in local potential fluctuations. The PL results are compared with highly spatially resolved cathodoluminescence directly visualizing the Cd-fluctuations and the phase separation.

HL 26.4 Tue 16:00 POT 51

Whispering gallery modes in hexagonal nanocavities – theory vs. experiment. — •Thomas Nobis, Andreas Rahm, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Linnéstraße 5, D-04103 Leipzig

Concerning nano-photonics, zinc oxide (ZnO) nanostructures are frequently envisioned as resonator cavities in future optical devices, such as nanolasers. Thus, a precise understanding of their optical modes is strongly necessary. In this work we analyzed the lateral optical modes, so-called whispering gallery modes (WGMs), of ZnO nanopillars grown by pulsed laser deposition with diameters around 800 nm. The regular hexagonal cross-section of the pillars naturally defines a two-dimensional (2D) dielectric cavity with the light circulating inside being totally internally reflected. Our analysis includes detailed numerical simulations of hexagonal WGMs solving the 2D Helmholtz-equation with respect to resonant wave numbers, line widths, mode patterns, polarization, mode degeneracy and spectral dispersion. Utilizing our numerical results we are able to simulate characteristic resonance lines of individual ZnO nanopillars in perfect agreement with the experiment [1]. As a result we can extract the birefringence of single pillars out of their WGM spectrum. Hence, the whispering gallery effect has been utilized to detect optical constants of nano-sized samples.

[1] Th. Nobis and M. Grundmann, Phys. Rev. A, in press

HL 26.5 Tue 16:15 POT 51

MOCVD-Growth of Arsenic and Nitrogen (dual)-doped epilayers: structural, electrical and optical properties — •Sören Giemsch, Armin Dadgar, Andre Krtschil, Frank Bertram, Jürgen Christen, and Alois Krost — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

The direct semiconductor ZnO with a large band-gap of 3.3 eV at room temperature and a binding energy of 60 meV for the free exciton offers great potential for inexpensive optoelectronic devices in the blue and near UV spectral region. Despite numerous research activities over the last years, reproducible and long-time-stable p-type ZnO is still difficult to achieve. Nitrogen at an oxygen-site and arsenic are potential candidates for the realisation of acceptor levels in ZnO and thereby p-type-conductivity. In scanning-capacitance-microscope measurements the long-time-stable p-type behaviour of MOCVD-grown nitrogen and arsenic dual doped ZnO-epilayers was shown [1]. Here we show further investigations of As-mono-doped and N / As-dual-doped MOCVD-grown ZnO-layers. The structural, electrical and optical properties of the epilayers grown under different AsH_3- and UDMHy-flows will be compared. [1]: A. Krtschil, A. Dadgar, N. Oleynik, J. Bläsing, A. Diez, and A. Krost, *Local p − type conductivity in zinc oxide co − doped with nitrogen and arsenic*, APL, to be published

HL 26.6 Tue 16:30 POT 51

Photoluminescence investigations on a native donor in ZnO — •Joachim Sann, Niklas Volbers, Stefan Lautenschläger, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

The shallow donor impurities in ZnO with binding energies between 46 and 56 meV have been studied in great detail in the recent years. They give rise to neutral donor bound exciton recombinations with the A- and B-valence bands, show rotator states and two-electron-satellite transitions. These properties allowed to establish the excited state splittings of the donors as well as confirming Hayne's rule in ZnO. So far they all seem to be of extrinsic origin, hydrogen, aluminum, gallium and indium in order of increasing binding energy. For many years it was common sense that intrinsic defects would dominate the n-type conductivity of ZnO. Interstitial zinc as well as oxygen vacancies should be double donors, and in order to contribute to the n-type-conduction they should have shallow levels, and low formation energies to be abundant. Undoped Zn-rich epitaxial films grown by CVD on GaN/Sapphire-templates as well as on ZnO templates show a dominant I_{3a} recombination at 3.367 eV in low temperature PL which according to Haynes rule is consistent with a shallow donor level at 37 meV. Moreover, they have free n-type carrier densities of $8x10^{18}$ cm^{-3} and as revealed by SIMS the common donor impurities (Al, Ga, In) cannot account for the high carrier densities. By changing the Zn/O ratio towards oxygen rich conditions the I_{3a} recombi-

nation is suppressed, a similar effect is found when annealing in oxygen atmosphere.

HL 26.7 Tue 16:45 POT 51

Fe^{2+} in ZnO studied by Fourier-transform transmission spectroscopy — •Enno Malguth[1], Axel Hoffmann[2], Matthew Phillips[1], and B. Hausmann[2] — [1]Microstructural Analysis Unit, University of Technology, Sydney, Australia — [2]Institut für Festkörperphysik, Technische Universität Berlin, Germany

ZnO crystals, coated with a 1 μm thick Fe layer and subsequently annealed under different atmospheres were studied by means of Fourier-transform infrared (FTIR) transmission spectroscopy. At 50 K, a pronounced absorption structure was detected around 395 meV exhibiting at least five distinct lines. Even at room temperature, a broad peak centered around 400 meV was observed. We attribute this absorption feature to the internal $^5E \longrightarrow {}^5T_2$ transition of the isolated Fe^{2+} center. This transition has been thoroughly studied in several cubic III-V and II-VI semiconductor materials, where it was found at similar energetic positions. However so far, it has not been established satisfactorily in ZnO where a crystal field of c_{3V} symmetry causes an additional splitting of the involved electronic states. By means of polarized measurements the observed lines are tentatively assigned to single transitions between ^5E and $^5T_2$ sublevels according to transition rules.

HL 26.8 Tue 17:00 POT 51

Hyperfine splitting in hydrogenated ZnO measured by electron spin resonance — •Marc A. Gluba, Felice Friedrich, and Norbert H. Nickel — Hahn-Meitner-Institut Berlin, Abteilung Silizium-Photovoltaik, Kekuléstraße 5, D-12489 Berlin

The source of the natural n-type doping of zinc oxide single crystals is still not completely clarified. However, hydrogen as an indispensable permanent impurity plays a crucial role. To elucidate the importance of hydrogen X-band electron spin resonance (ESR) measurements were performed on zinc oxide single crystals before and after hydrogenation. Hydrogen was introduced by annealing the samples for two hours at 830°C in sealed ampoules under hydrogen atmosphere. The ESR-measurements were performed at 5K.

As-grown zinc oxide exhibits a single ESR line arising from two shallow donors with similar g-values ($g_{||} = 1,957$, $g_{\perp} = 1,956$). One of which was identified as hydrogen [1]. On the other hand, hydrogenated zinc oxide shows distinctly different ESR spectra. Besides the intensification of the donor related line a variety of new features in a broad range of about 1000G around the center line is observed. These are likely to arise from hyperfine interaction between electrons of neutralized hydrogen donors and adjacent ^{67}Zn nuclei of spin 5/2. Based on the performed experiments conclusions on the position of the hydrogen centers in the ZnO lattice can be drawn.

[1] Detlev M. Hofmann et al., Phys. Rev. Lett., **88** no. 4, 045504 (2002)

HL 26.9 Tue 17:15 POT 51

First-principles study of migration mechanisms and diffusion of oxygen in zinc oxide — •Paul Erhart and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 23, 64287 Darmstadt

We have performed density-functional theory (DFT) calculations in conjunction with the climbing image-nudged elastic band method (CI-NEB) in order to study the self-diffusion of oxgyen in zinc oxide. To this end, we have generalized the migration paths accessible for vacancies as well as interstitials in wurtzite crystals and derived expressions which provide the link to experimentally accessible tracer diffusion coefficients. The calculated migration barriers are consistent with annealing experiments on irradiated samples. We find that vacancy and interstitialcy mechanisms dominate under zinc and oxygen-rich conditions, respectively. Either mechanism can in principle lead to the experimentally observed diffusivities. However, diffusion experiments are normally carried out in oxygen atomosphere and will, therefore, sample oxygen interstitial diffusion. Our results provide the basis for the (re-)interpretation of previous and future diffusion experiments, and pave the way towards the development of reliable continuum models for device simulation.

HL 26.10 Tue 17:30 POT 51

A comparative study of the substrate influence on the structure of pulsed laser-deposited ZnO thin films — •Felice Friedrich, Ina Sieber, and Norbert H. Nickel — HMI Berlin, Abt. SE1, Kekuléstr. 5, D-12489 Berlin

Nominally undoped ZnO thin films were deposited by pulsed laser deposition (PLD) on different substrates, namely silicon, quartz, sapphire, and magnesium oxide. For better comparability ZnO was grown on all substrates simultaneously. The thickness of the resulting ZnO layers was about 1 μm. The chamber pressure was varied between 10^{-3} mbar and 3 mbar depending on the oxygen flow whereas the deposition temperature was held constant at 700°C. The films were characterized using SEM and Raman backscattering spectroscopy.

With increasing pressure a transition from ZnO thin films to the formation of nanostructures was observed. Furthermore a strong influence of the substrate on the layer orientation and the degree of disorder in the ZnO films has been found. This is likely due to the respective lattice mismatch. Raman spectra of the films on quartz substrates show the recently controversially discussed additional local vibrational modes that were observed in doped ZnO thin films and amongst others related to the presence of nitrogen [1]. However, in connection with the SEM results we tend to assign these modes to disorder activated Raman scattering of the silent B_1 modes in ZnO [2]. This will be discussed in detail.

[1] Haboeck et al., PSS (b) 242 (2005) R21
[2] Manjón et al., JAP 97 (2005) 053516

HL 26.11 Tue 17:45 POT 51

Optical and electrical properties of phosphorous doped ZnO thin films — •M. Grundmann[1], H. von Wenckstern[1], J. Sann[2], M. Brandt[1], G. Benndorf[1], S. Heitsch[1], A. Krtschil[3], M. Lorenz[1], B. K. Meyer[2], and A. Krost[3] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig — [2]I.Physikalisches Institut JLU-Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen — [3]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, PO Box 4120, 39016 Magdeburg

ZnO is a wide band-gap semiconductor with remarkable material properties. First and foremost the large excitonic binding energy of about 60 meV makes ZnO interesting for UV optoelectronic applications. The major obstacle nowadays is the difficulty of reproducibly growing high quality p-type ZnO. We have investigated the properties of ZnO thin films doped with phosphorous. The samples are grown by pulsed-laser deposition on sapphire or ZnO single crystalline substrates. The optical properties are investigated by means of recombination spectra. Integral electrical properties are obtained from Hall effect measurements. The Fermi level close to the surface is determined by scanning surface potential microscopy. Possible lateral dependencies of the net doping density are investigated by scanning capacitance microscopy, showing p-type domains for homo-epitaxially grown ZnO:P, for instance. Independent on the growth conditions the samples show a pronounced correlation between the resistivity and with that the Fermi level and the intensity ratio between the near band edge and deep level emission.

HL 26.12 Tue 18:00 POT 51

Electrical characterization of deep acceptor states in N implanted ZnO single crystals — •H. von Wenckstern[1], H. Schmidt[1], R. Pickenhain[1], G. Biehne[1], M. Brandt[1], G. Brauer[2], M. Lorenz[1], and M. Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig — [2]Institut für Ionenstrahlphysik und Materialforschung, FZ Rossendorf, Postfach 510119, D-01314 Dresden

ZnO is investigated again in the past few years with enormous effort due to, e.g., the availability of ZnO substrate material or the promising material properties of ZnO such as the high exciton binding energy or the radiation hardness. Up to now, several deep electron traps in ZnO have been characterized electrically. To our knowledge there do not exist any reports concerning elctrical characterization of deep acceptor-like states in ZnO. We report in this contribution on acceptor-like states in ZnO investigated by deep level transient spectroscopy (DLTS). For that, a ZnO single crystal was implanted by N^+ ions using an acceleration voltage of 150 keV. The crystal was annealed prior to the electrical characterization for 30 min at 500°C in an oxygen ambient to reduce damage caused by implantation. Scanning capacitance microscopy measurements on the implanted side of the sample revealed p-type conduction. With that, the observation of both electron and acceptor-like defects is possible. The DLTS measurements confirmed the existence of the electron traps E3 and E4. Additionally, we were for the first time able to characterize a deep acceptor state labelled W2. The thermal activation energy of W2 is estimated to be 260 - 280 meV.

HL 26.13 Tue 18:15 POT 51

ZnO films doped with rare earth metals — •M. Diaconu[1], H. Schmidt[1], H. Hochmuth[1], H. von Wenckstern[1], D. Spemann[1], M. Lorenz[1], M. Grundmann[1], M. Fecioru-Morariu[2], K. Schmalbuch[2], and G. Güntherodt[2] — [1]Inst. für Exp. Physik II, Fakultät für Physik, Uni. Leipzig, Linnestrasse 3-5, 04103 Leipzig — [2]II. Physikalisches Institut, RWTH Aachen, Physikzentrum Melaten, Huyskensweg Turm 28B, 52074 Aachen

The electrical and magnetic properties of ZnO:Gd and ZnO:Nd were studied for films grown by pulsed laser deposition on *a*-plane sapphire. Different growth conditions were used to prepare ZnREO films with RE = Gd or Nd contents around 0.01, 0.1 or 1 at% and thicknesses from 50 nm to 1000 nm. The rare earth concentration and position in the wurtzite lattice were determined by Rutherford backscattering and particle induced X-ray emission. Hall investigations revealed a dependence of the electrical properties on film thickness and composition. Magnetic properties were investigated in a wide temperature range using a superconducting quantum interference device and magneto-optical Kerr effect.

HL 26.14 Tue 18:30 POT 51

Optical characterisation of ZnO nanostructures grown by various methods — •Chegnui Bekeny[1], Houcem Gafsi[1], Tobias Voss[1], Bianca Postels[2], Marc Kreye[2], Sandra Börner[3], and Wolfgang Schade[3] — [1]Institute of Solid State Physics, University of Bremen, P.O Box 330440, D-28334 Bremen — [2]IHT, TU Braunschweig, P.O Box 3329, D-38023 Braunschweig — [3]IPPT, TU Clausthal, Leibnizstraße 4, D-38678, Clausthal-Zellerfeld

ZnO, a semiconductor with a band gap of 3.37 eV, is currently in the focus of research due to its relatively large exciton binding energy of 60 meV and its ability to emit light in the uv spectral region. In order to integrate ZnO nanostructures into optoelectronic devices, it is imperative to thoroughly understand their optical properties. We present systematic photoluminescence studies of ZnO nanorods fabricated by aqueous chemical growth (ACG). These nanorods show significant near band-edge excitonic luminescence accompanied by very little green and orange defect luminescence. In combination with distinct phonon replica of the excitonic lines observed this indicates a good optical quality of the ACG nanorods. The optical properties of nanorods grown on different substrates (Si and plastic foil) will be compared with ZnO nanostructures grown by other epitaxial methods. Additional investigations concerning possible laser action in ZnO nanowires were performed using vapour-liquid-solid grown nanowires. At high excitation densities (>0.5 MW/cm*) single nanowires (dispersed on a sapphire substrate) showed a narrow emission line at ˜3.2 eV (line width 0.5 meV) even at room temperature.