HL 9: ZnO: Preparation and characterization I

Time: Monday 15:00–18:30 Location: EW 201

HL 9.1 Mon 15:00 EW 201

Magnetische und Strukturelle Untersuchung von Mangan-dotierten Zinkselenid-Halbleiternanopartikeln — •Andreas Hofmann[1], Christina Graf[1], Thomas Ackermann[2], Christine Boeglin[3], Xiaogang Peng[4], Ranjani Viswanatha[4], Arantxa Fraile-Rodriguez[5], Frithjof Nolting[5] und Eckart Rühl[1] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin — [2]Institut für Physikalische Chemie, Universität Würzburg, 97074 Würzburg — [3]Institute de Physique et Chimie des Materiaux de Strasbourg, 67034 Strasbourg — [4]Department of Chemistry and Biochemistry, University of Arkansas, 72701 Fayetteville — [5]Paul Scherrer Institut, SLS, 5232 Villigen

Mn-dotierte ZnSe Nanopartikel sowie ZnSe-Partikel mit einem MnSe-Kern wurden mit chemischen Hochtemperaturverfahren synthetisiert. Die Mn-Konzentration betrug dabei $0.2 - 5\%$ bei einer Partikelgröße von $2.8 - 7.5$ nm. Um die elektronische Struktur und die magnetischen Eigenschaften der Mangan-Atome näher zu untersuchen, wurden an den Nanopartikeln magnetische Röntgenzirkulardichroismus-Messungen (XMCD) durchgeführt. Dabei konnte für alle Proben gezeigt werden, dass die Mn-Atome im Inneren der Nanopartikel lokalisiert sind und nicht oxidiert vorliegen. Die Polarisierung der Mn-Atome beträgt im Falle der isolierten Mn-Atome bis zu 80% des theoretischen Wertes eines freien d^5-Zustandes. Die Partikel mit einer MnSe/ZnSe Kern-Schale-Struktur zeigen in Abhängigkeit der Mn-Konzentration eine verminderte Polarisierung von etwa 50%.

HL 9.2 Mon 15:15 EW 201

ZnO-nanowire as a nanogenerator? — •Markus Andreas Schubert, Stephan Senz, Marin Alexe, and Ulrich Gösele — Max Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

Recently nanogenerators for powering nanodevices were reported [1] in which ZnO-nanowire arrays convert mechanical energy in electrical energy by bending the ZnO-nanowires.

We simulate the experiments in which the ZnO nanowires were bent by AFM tip [2] by FEM-calculations for an ideal nonconducting piezoelectric ZnO-nanowire with a length of 600 nm and a diameter of 50 nm fixed perpendicular to a substrate. The top part of this nanowire was bent about 140 nm by a force applied at the top of the nanowire. At the point of the applied force the electrical potential has a maximum of +1.3 V. In the rest of the nanowire the electrical potential is +0.3 V for the stretched side and -0.3 V for the compressed. The piezoelectric charge generate the signal on the capacitance between the two sides, which is about 10^{-5} pF for the whole wire. A lower value of 10^{-7} pF is estimated for the AFM point contact.

However, most ZnO-nanowires are n-doped semiconductors with a typically resistivity of 1 Ωcm. One consequence is a very fast discharging of the piezoelectric generate charge in the order of magnitude of 1 ps. Even, in the case of an ideal nonconducting nanowire, the voltage at the input capacity of any preamplifier (∼1-5 pF) would be of the order of 10^{-7} V, which corresponds to a charge of about one electron.

[1] Y. Gao and Z.L. Wang, Nano Letters **7**, 2499–2505 (2007)
[2] Z.L. Wang and J. Song, Science **312**, 242–246 (2006)

HL 9.3 Mon 15:30 EW 201

Homoepitaxial growth of ZnO thin film by pulsed laser deposition (PLD) — •Matthias Brandt[1], Holger von Wenckstern[1], Holger Hochmuth[1], Michael Lorenz[1], Gisela Biehne[1], Gabriele Benndorf[1], Christoph Meinecke[1], Tilman Butz[1], Heidemarie Schmidt[1,2], Andreas Rahm[1,3], and Marius Grundmann[1] — [1]Universität Leipzig, Semiconductor Physics Group, Institut für ExperimentellePhysik II, Leipzig, Germany — [2]now at Forschungszentrum Dresden–Rossendorf, Dresden, Germany — [3]now at Solarion AG, Leipzig, Germany

Homoepitaxy has proven to improve the structural quality of ZnO thin films considerably compared to heteroepitaxy [1]. In this work the transport properties of phosphorous doped ZnO thin films, grown by pulsed–laser deposition (PLD) on thermally pretreated hydrothermally grown ZnO single crystal substrates are reported. Atomic force microscopy (AFM), high resolution X–ray diffraction and Rutherford backscattering (RBS) channeling measurements have been employed to analyse the morphological and structural properties of the ZnO:P thin films. Steps of height $c/2$ are visible in AFM images of all samples. For an oxygen partial pressure of 0.1 mbar two–dimensional growth was found. RBS–Channeling of a ZnO:P film shows a minimum yield of 0.034 which is comparable to that of an annealed substrate (0.033). Hall effect measurements revealed that all as–grown ZnO:P thin films are n–type. Peak mobilities of 800 cm^2/Vs have been observed around 70 K, being in line with the high structural quality of the samples.

[1] H. v. Wenckstern et al.: phys. stat. sol. (RRL) **1**, 129 (2007).

HL 9.4 Mon 15:45 EW 201

Cathodoluminescence on homoepitaxially grown phosphorus doped ZnO epilayers — •Jan Zippel, Holger von Wenckstern, Gabriele Benndorf, Matthias Brandt, Michael Lorenz, Christoph Meinicke, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

Phosphorus doped ZnO thin films were grown homoepitaxially by pulsed-laser deposition (PLD). The hydrothermal ZnO substrates were heat treated in oxygen ambient (850 mbar) at 1000°C for 2 h which results in a vicinal surface perfectly suited for epitaxy [1]. PLD-targets with different content of phosphorus were used(1 wt.%, 0.1 wt.%, 0.01 wt.%) for thin film deposition. Additionally we change the oxygen partial pressure systematically from 0.0003 mbar to 0.1 mbar. All samples were annealed (800 W, 10 min, 700 mbar N2).

In this contribution we compare low temperature (10K) cathodoluminescence (CL) of the as-grown and the annealed state in dependence on the phosphorus content and the oxygen partial pressure. Typical CL spectra are dominated by peaks related to the band edge and peaks related to deep impurities, respectively. We find that the red band dominates the spectra for high oxygen partial pressure independent of the phosphorus content whereas the green band is significant for low oxygen partial pressure and high phosphorus content.

[1] H. von Wenckstern, H. Schmidt, C. Hanisch, M. Brandt, C. Czekalla, G. Benndorf, G. Biehne, A. Rahm, H. Hochmuth, M. Lorenz and M. Grundmann, phys. stat. sol. (RRL) {1}, 129 (2007)

HL 9.5 Mon 16:00 EW 201

Structural and electronic properties of ZnO nanowires and nanotubes — •Andreia Luisa da Rosa[1], Hu Xu[2], Wei Fan[2], Fei Zhan[2], Xiaohong Zhang[2], Ruiqin Zhang[3], and Thomas Frauenheim[1] — [1]BCCMS, Universität Bremen, Am Fallturm 1, 28359, Bremen, Germany — [2]Nano-organic Photoelectronic Laboratory, Technical Institute of Physics and Chemistry, Beijing 100101, China — [3]COSDAF, Department of Physics and Materials Science, City University of Hong Kong SAR, China

ZnO is a well known semiconductor with potential applications in electronics and optoelectronics. ZnO has a direct wide band gap of 3.3 eV and a large exciton binding energy making it promising for high-efficiency blue and ultra-violet devices. Recently, the successful growth of highly ordered nanowires has expanded the list of potential applications. In this work we employ density functional theory to investigate ZnO nanowires and nanotubes. We find that relaxations on the facets are very similar to the ones in non-polar ZnO surfaces. While bare and completely passivated wires are semiconducting, wires with intermediate hydrogen passivation exhibit metallic behavior. We therefore suggest that hydrogenation leads to drastic changes in the ZnO nanowire electrical properties. We have also investigated ZnO nanotubes with round and hexagonal shapes. The calculated strain energy of round ZnO nanotubes follows a classical strain law. All the ZnO nanotubes were found to be direct band gap semiconductors with the band gap decreasing as their diameter increases.

HL 9.6 Mon 16:15 EW 201

Growth and doping of ZnO — •Stefan Lautenschläger, Joachim Sann, Niklas Volbers, Jan E. Stehr, Andreas Laufer, Thomas Leichtweiss, and Bruno K. Meyer — I.Physikalisches Institut, Justus Liebig Universität Gießen, Deutschland

The so far not reliably resolved acceptor doping of ZnO is clearly the main obstacle for the successful development of working devices based on ZnO. We report on the possibilities of acceptor doping during the CVD growth of ZnO. To achieve the incorporation of an acceptor we used the group V elements arsenic and nitrogen. We investigated mainly epitaxially grown thin films, some comparison with Ion- im-

planted samples have been undertaken. All the samples have been analyzed using photoluminescence spectroscopy, secondary ion mass spectrometry, atomic force microscopy, X-Ray photoelectron spectroscopy (XPS) and scanning electron microscopy. Especially the As- doped and implanted samples have been investigated with XPS to obtain information about the lattice site the dopant occupies.

15 min. break

HL 9.7 Mon 16:45 EW 201

Thermal and flash lamp annealing of nitrogen–implanted ZnO thin films. — •Thomas Lüder[1], Christian Czekalla[1], Gabriele Benndorf[1], Matthias Schmidt[2], Wolfgang Anwand[2], Gerhard Brauer[2], Wolfgang Skorupa[2], Manfred Helm[2], and Marius Grundmann[1] — [1]Universität Leipzig, Leipzig, Germany — [2]Forschungszentrum Dresden – Rossendorf e.V., Dresden, Germany

pn–junctions in ZnO have already been built by implantation of nitrogen ions. Post–annealing methods are used in order to activate the N_O acceptor and reduce defects caused by implantation processes. However out–diffusion of nitrogen during thermal annealing reduces the acceptor concentration and might lead to a loss of p–type conductivity. Recent success in using flash lamp annealing on Fe implanted ZnO single crystals[1] encouraged us to apply this post–annealing method to nitrogen–implanted ZnO thin films grown by pulsed laser deposition on sapphire substrates. The short annealing time of this process should minimize the diffusion of nitrogen.

Our samples have been annealed under three different flash lamp annealing conditions and are compared to thermally annealed samples.

The samples have been investigated by electrical and optical methods. We used low temperature photoluminescence and Raman–spectroscopy to prove the incorporation of nitrogen on oxygen sites. To finally get results of the electrical activity of the N_O acceptors, the samples have been examined by current–voltage measurements.

[1] K. Potzger et al.: J. Appl. Phys. **101**, 033906 (2007).

HL 9.8 Mon 17:00 EW 201

Hydrogen motion in the Cu-H complex in ZnO — •Felix Börrnert, E. V. Lavrov, and J. Weber — Technische Universität Dresden, 01062 Dresden, Germany

The Cu-H complex in ZnO consists of Cu on Zn site and a hydrogen atom bound to a nearby O atom with the O–H bond oriented in the basal plane of the hexagonal lattice to the c axis. The motion of hydrogen in the Cu-H complex is studied by the stress-induced dichroism. Stress applied at room temperature along $[10\bar{1}0]$ results in an alignment of the Cu-H bond. The reorientation process was found to be thermally activated with the activation energy of 0.52 ± 0.04 eV. The connection of the hydrogen movement in the Cu-H complex with the hydrogen diffusion in ZnO is discussed and consequences for the existence of interstitial hydrogen in ZnO at room temperature are presented.

HL 9.9 Mon 17:15 EW 201

Sputtered Silver Contacs on Zinc Oxide — •A. Lajn, H. von Wenckstern, M. Schmidt, M. Brandt, G. Biehne, H. Hochmuth, M. Lorenz, and M. Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für ExperimentellePhysik II, Leipzig, Germany

Rectifying metal-semiconductor contacts are an adequate tool for investigating the electrical properties of semiconductors by means of, e.g., current-voltage- (IV) or capacitance-voltage-characterisation (CV) or thermal admittance spectroscopy (TAS). Reactive sputtering of silver in an oxygen atmosphere is a reproducible method to realize contacts on zinc oxide single crystals with excellent rectification properties [1]. In this contribution we investigate the properties of such contacts on hydrothermally grown ZnO bulk single crystals and on ZnO thin films grown by pulsed-laser deposition (PLD). The contacts realized on PLD thin films have a rectification ratio I(1V)/I(-1V) of 10^6, the typical rectification ratio for contacts on bulk crystals is 10^5. Both IV and CV characteristics confirm the formation of Schottky contacts. The barrier heights are about 0.9 V and the ideality factors are below 1.3 for thin films and about 1.6 for single crystals. Further the contact properties were investigated by temperature-dependent IV measurements confirmimg the usability of the contacts for semiconductor defect characterisation. As example TAS measurements on various electronic defects are presented.

[1] M. W. Allen, S. M. Durbin and J. B. Metson, Appl. Phys. Lett. **91**, 053512 (2007).

HL 9.10 Mon 17:30 EW 201

Implantationsuntersuchungen an polaren und unpolaren ZnO Einkristallen — •Patrick Kessler und Reiner Vianden — Helmholtz- Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn

Untersucht wurden in verschiedene Richtungen orientierte ZnO Kristalle mit der Methode der gestörten γ - γ Winkelkorrelation (PAC). Dabei wurden die Kristalle mit ^{111}In als Sondenatomen dotiert, die bevorzugt auf Zink Gitterplätze eingebunden werden. Deren direkte Umgebung kann mit der gewählten Messmethode dadurch hochaufgelöst studiert werden.

Um einen möglichen Effekt der Polarität und der daraus resultierenden Oberflächenterminierung auf das Ausheilverhalten der Implantationsschäden zu untersuchen wurde ein vergleichendes isochrones Temperprogramm an $\langle 0001 \rangle$, $\langle 10\bar{1}0 \rangle$ und $\langle 11\bar{2}0 \rangle$ orientierten ZnO Einkristallen durchgeführt.

HL 9.11 Mon 17:45 EW 201

Properties of Li doped ZnO nanocrystals prepared from organometallic precursors — •Christian Rauch[1], Markus R. Wagner[1], Ronny Kirste[1], Wolfgang Gelhoff[1], Axel Hoffmann[1], Michael Lehmann[1], Matthias Driess[1], Andrey Orlov[2], and Sebastian Polarz[2] — [1]Technische Universität Berlin — [2]Universität Konstanz

Applying a special organometallic precursor system, ZnO nanocrystals with considerable Li incorporation were produced. The structural, optical and electronic properties of the Li doped ZnO nanocrystals with lithium concentrations between 0.1 and 12 percent are studied by x-ray diffraction (XRD), photoluminescence (PL) and electron paramagnetic resonance (EPR) spectroscopy. The XRD patterns demonstrate that ZnO solely crystallises in the wurtzite structure, with no other phases present. The ZnO particles are of similar size (70-80nm) with no considerable strain. However, a deviation of the lattice parameters for Li containing ZnO samples could be observed. The incorporation of lithium in the lattice, the g-values and the charge transfer processes are studied by photo-excited EPR. The successful lithium incorporation on the Zn site leads to a reduction of the Fermi level compared to undoped ZnO. The PL spectra at helium temperature show a bound exciton transition in the range of I_8, a luminescence band around 3.31eV with strong dependence on the Li concentration and a significant donor-acceptor-pair luminescence for medium lithium concentrations. The experimental data are discussed concerning the effectiveness of the shallow Li acceptor towards p-conductive ZnO nanocrystals.

HL 9.12 Mon 18:00 EW 201

ZnO nanocolumns grown by catalyst-free plasma assisted molecular beam epitaxy — •Thomas Andreas Wassner, Bernhard Laumer, Stefan Maier, Jochen Bruckbauer, Martin Stutzmann, and Martin Eickhoff — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

ZnO nanocolumns were grown on (11-20)-sapphire by plasma assisted molecular beam epitaxy without the use of a catalyst. The influence of the II-VI ratio and the substrate temperature during growth on the density and shape of the nanocolumns was investigated. The epitaxial relationship was found to be $Al_2O_3[0001] \| ZnO[11\text{-}20]$, as determined by high resolution X-ray diffraction. Transmission electron microscopy images and Raman measurements will be presented in order to discuss the structural quality of the ZnO-nanorods. Optical properties, probed by photoluminescence spectroscopy are compared with those of continuous ZnO epitaxial films.

HL 9.13 Mon 18:15 EW 201

Chemical nature of N incorporated into ZnO during epitaxial film growth — •Patrick Hoffmann, Christian Pettenkofer, and Stefan Andres — Hahn-Meitner-Institut, Glienicker Straße 100, 14109 Berlin

ZnO is a wide band gap semiconductor (gap=3.4eV) which is unintentionally n doped by nature. In the last years it has been shown that ZnO can be p doped by incorporation of nitrogen. Nevertheless, some puzzling results suggest that just incorporation of nitrogen not simply leads to p doped ZnO. Investigations have shown that nitrogen can replace oxygen (N_O, p doping), but can also be incorporated as molecular N_2 ($[N_2]_O$, n doping), and can be bonded to oxygen. Therefore, this investigation concentrates on the chemical nature of the incor-

porated nitrogen during ZnO growth. The ZnO films are grown by metal-organic MBE (MOMBE) on sapphire substrate (r plane), while nitrogen is supplied by an ion source. Additionally, a mass filter between the ion source and the sample gives the opportunity to minimise the influence of the neutrals (e.g. N_2), and to select certain ions and ion fractions (e.g. N_2^+, N^+). The obtained films were investigated by means of XPS and NEXAFS. A comparison of the differently prepared films will be given.