HL 38: ZnO and Related Semiconductors

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

HL 38.1 Wed 9:30 H17

Surface structure and excitonic transitions of ZnO single crystals for homoepitaxy — •Daniel Fritsch[1], Olga Roshupkina[2], Jörg Grenzer[2], and Heidemarie Schmidt[2] — [1]School of Physics, Trinity College Dublin, Ireland — [2]FZD, Institute of ion beam physics and materials research, Germany

The surface quality and mosaicity of as received ZnO single crystals strongly depends on the applied crystal growth and subsequent surface polishing techniques. As a result single crystallite ZnO substrates are very often build up as a complex of single crystallite columnar structures. This microcrystalline substrate structure strongly influences the preparation of high-quality homoepitaxial ZnO films [1].

The columnar vs. mosaicity structure of as received Zn- and O-polar polished surfaces and unpolished backsides of (0001) ZnO substrates has been evidenced from high-resolution x-ray diffraction of the (0004) and $(11\bar{2}4)$ reflections and from atomic force microscopy analyses. It was shown that there is a weak increase of the c-lattice parameter due to the polishing. The strain, induced by polishing, is evaluated from the probed c-and a-lattice parameter and used as an input parameter for emipirical pseudopotential (EPM) [2] calculations including excitonic effects near the direct bandgap. The calculated strain-dependent optical absorption near the direct band gap of ZnO has been related with the optical properties of the polished surfaces of ZnO single crystals probed in the spectral region from 1 to 4 eV using a VASE spectral ellipsometer. [1] H. von Wenckstern et al., phys. stat. sol. (RRL) 1, 129-131 (2007). [2] D. Fritsch, PhD thesis, Engelsdorfer Verlag, 2007.

HL 38.2 Wed 9:45 H17

Patterned growth of ZnO nanopillars — •Manfred Madel, Yong Xie, Martin Feneberg, Thilo Zoberbier, Benjamin Neuschl, Uwe Röder, and Klaus Thonke — Institut für Halbleiterphysik, Universität Ulm

To get a regular hexagonal arrangement of ZnO nanopillars on sapphire substrate, self-assembling monolayers of polystyrene (PS) spheres are used to cover a-plane sapphire substrates on which gold or nickel catalysts are deposited. We employ wet-chemical etching to remove the catalyst regions not protected by the PS. After lift-off of the colloid spheres a well prepatterned catalyst structure is obtained as confirmed by atomic force measurements. After optimizing the growth conditions ZnO nanopillars with diameters between 200 and 500 nm and lengths up to 5 μm are grown in hexagonal arrays on areas larger than 1 mm^2. Photoluminescence measurements show a perfect crystal quality with a full width at half maximum below 250 μeV for donor bound exciton lines in ZnO.

HL 38.3 Wed 10:00 H17

Gain dynamics of single ZnO nanowires — •Jan-Peter Richters, Jürgen Gutowski, and Tobias Voss — Institute of Solid State Physics, University of Bremen, P.O. Box 330440, D-28334 Bremen

Nanostructures of large band-gap semiconductors like ZnO are of great interest as light emitting and lasing media in the blue-UV spectral range. In order to use ZnO nanowires as lasing devices it is important to understand the spectral and temporal characteristics of their material and modal gain. Theoretical calculations predict a very high modal gain close to the material gain for semiconductor nanowires which is due to the very high confinement of the light for such nanostructures.

We investigate the gain of single ZnO nanowires under excitation with fs-laser pulses from a frequency tripled regenerative amplifier (800 nm, pulse duration less than 100fs, repetition rate 1kHz, pulse power 3 mJ) using the variable-stripe-length method allowing for the investigation of the profile of their modal gain. The measurements are carried out at room temperature on a glas substrate. We ammount the modal gain to 6000 - 8000 cm^{-1} for nanowires with diameters larger than 200 nm. These results are in good agreement with theoretical predictions from the literature where a values of up to 2500 cm^{-1} for GaN nanowires with a diameter of 105nm has been calculated.

HL 38.4 Wed 10:15 H17

Light-emitting devices based on ZnO-nanowire arrays coated with p-conductive polymers — Abdelhamid Elshaer, Apurba Dev, Jan-Peter Richters, and •Tobias Voss — Institut für Festkörperphysik, Universität Bremen

Due to their large surface-to-volume ratio and high crystalline quality, ZnO nanowires are promising candidates for optoelectronic applications in the blue-UV spectral region. Especially low-temperature grown ZnO nanowires offer interesting properties for the large-scale and low-cost production of environmentally friendly solar cells and light-emitting diodes. When a p-conductive polymer is used to form a hybrid junction, stable UV emission from such a heterojunction has also been observed. We have employed a wet-chemical synthesis method to fabricate ZnO nanowire arrays on conductive glass substrates. The typical dimensions of the nanowires are about 100 nm in diameter and 2 μm in length. A thin layer of the polymer PEDOT:PSS was spin-coated onto the nanowires to fabricate compound structures acting as light emitting diodes. We studied the electroluminescence and the I-V-characteristics of the devices for different polymers and processing parameters. An additional insulating polymer layer (polystyrene) coated directly onto the nanowires was found to significantly improve the device characteristics. This is in agreement with our previous investigations of n-ZnO nanowire/p-silicon light emitting diodes where an insulating silicon dioxide layer between the n-ZnO and the p-silicon is needed to allow for tunnel injection of holes into the ZnO valence band.

HL 38.5 Wed 10:30 H17

Stable enhancement of near band edge emission of ZnO nanowires by hydrogen incorporation — •Apurba Dev[1], Raphael Niepelt[2], Jan Peter Richters[1], Carsten Ronning[2], and Tobias Voss[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Solid State Physics, University of Jena, Germany

ZnO nanowires have drawn considerable interest as efficient nanoscale UV light emitting device. However, due to the presence of defect states in the band gap, most of the radiative transitions take place via defect channels giving rise to a strong visible luminescence. At the same time, the near-band-edge emission is reduced. Several attempts have been made to increase the internal quantum efficiency of the UV emission by means of efficient energy transfer between surface plasmons of attached metal nanoparticles and the excitons in ZnO. In addition, passivation of the defect centers by incorporation of hydrogen impurities was also found to be a very effective way.

We performed a mild Ar plasma treatment on ZnO nanowires. The plasma-treated nanowires showed a stable and strong enhancement of the near-band-edge emission and a quenching of the deep-level emission. Photoluminescence studies at 4 K revealed a strong hydrogen donor-bound-exciton line in the plasma treated samples indicating unintentional incorporation of hydrogen. To confirm the results, hydrogen was implanted into the ZnO nanowires with a low ion energy of 600 eV and with different fluences. The observed result can be related to the passivation of deep centers by hydrogen.

HL 38.6 Wed 10:45 H17

Synthesis of different ZnO and other nanostructures by modified-VLS approach — •Yogendra Kumar Mishra[1], Sören Kaps[1], V S K Chakravadhanula[2], Seid Jebril[1], Lorenz Kienle[2], and Rainer Adelung[1] — [1]Functional Nanomaterials, Institute for Materials Science, Faculty of Engineering, Christian-Albrechts-University, Kaiserstrasse 2, 24143 Kiel, Germany — [2]Synthesis and Real Structures, Institute for Materials Science, Faculty of Engineering, Christian-Albrechts-University, Kaiserstrasse 2, 24143 Kiel, Germany

Nanostructures of zinc oxide which are a member of II-VI wide direct bandgap biocompatible semiconductor family, have been of immense fundamental and technological research investigation due to their unqiue optical, electrical and mechanical properties. Several methods have been used for controlled synthesis of different ZnO nanostructures but the fundamental growth mechanism is still an open issue. In present work we report a very simple modified-vapour liquid solid approach for the synthesis of ZnO nanorods, nanoseaurchins and nanocups. Growth mechanism in terms of concentration, temperature and environment will be discussed. Structural evolution of ZnO

nanorods and their elemental mapping using high resolution transmission electron microscopy will be presented. Formation of triangular, pentagonal, hexagonal gold nanoparticles and Au nanorods in ZnO matrix will also be presented. Modified vapour liquid solid approach in our group offers a very simple way to synthesize nanostructures of other metals and polymers and some of them will be shown and discussed.

15 Min. Coffee Break

HL 38.7 Wed 11:15 H17

Dynamics of the deep-level emission in ZnO nanowires — •Dongchao Hou, Ilja Rückmann, and Tobias Voss — Institut für Festkörperphysik, Universität Bremen

Due to its wide direct band gap and large exciton binding energy (60 meV), ZnO nanowires possess an efficient near band-edge emission (NBE) in UV range. Additional energy levels in the band gap of ZnO, commonly introduced by point defects such as oxygen or zinc vacancies and Cu impurities, can largely weaken the UV emission by providing extra recombination routes for the electrons in conduction band. In ZnO nanowires this deep-level emission band (DLE) is expected to be largely activated by tunneling processes of holes trapped in the surface depletion layer after optical excitation.

We studied the dependence of the DLE and NBE intensities of ZnO nanowires on the excitation power at different temperatures. For the experiments, the fundamental (1064 nm) and frequency-tripled (355 nm) pulses of an Nd:YAG microchip laser were used. The additional infrared laser radiation was used to directly populate the defect levels with electrons from the valence band. Our results show that the additional infrared photons lead to a reduction of the DLE while the NBE is enhanced. We will discuss the implications of our results for the models of DLE in ZnO nanowires.

HL 38.8 Wed 11:30 H17

First-principles DFT study of dopant elements at grain boundaries in ZnO — •Christian Elsässer and Wolfgang Körner — Fraunhofer Institut für Werkstoffmechanik, IWM, Freiburg, Germany

We present a first-principles density-functional-theory study of doped ZnO with focus on its application as a transparent conducting oxide (TCO). TCOs with high optical transparency and high electrical conductivity are for example applied in low emissivity windows, as transparent electrodes in photovoltaic cells or light emitting diodes. We investigated the impact of grain boundaries on the physics of atomic defects, and especially the formation energies of oxygen vacancies, cation dopants Al and Ga and anion dopants N and P are determined. The main goal is to obtain information about the positions of the defect levels generated by the different dopants in the electronic band gap. Because of the known deficiency of the local density approximation (LDA) to yield accurate values for band gap energies for insulators like ZnO a self-interaction correction (SIC) to the LDA is employed,which merely increase the computational costs. The main result of our study is that grain boundaries do affect the formation energies for substitutional dopants significantly. Furthermore the position and shape of dopant-induced electronic energy levels at the grain boundaries are changed considerably with respect to the single crystal. This may help to explain for example why N-doping can lead to p-conductivity at room temperature.

HL 38.9 Wed 11:45 H17

Excitons and their excitation channels in a-plane and c-plane ZnO — •Martin Kaiser[1], Markus R. Wagner[1], Gordon Callsen[1], Axel Hoffmann[1], S. Lautenschläger[2], S. Eisermann[2], and Bruno K. Meyer[2] — [1]Institut für Festkörperphysik, Technische Universität Berlin Germany — [2]Physikalisches Institut , Justus-Liebig-Universität Gießen, Germany

In the last decade ZnO inspired an experimental revival due to improvements in growth techniques and its potential for future devices like polariton lasers and spintronic materials. However, the growth of high quality ZnO and p-doping is still a big challenge. Optical characterizations of defects and excitons assist in the understanding of energy transfer processes and provide indications for the optimization of the growth parameters. We report on studies for a-plane and c-plane grown bulk ZnO. Compared to non-polar a-plane material [1120], ZnO has a strong piezoelectric field for polar growth along the c-direction [0001]. In this contribution, we present polarization dependent photoluminescence (PL) spectra in order to study the influence of the polarity on the radiative free and bound exciton recombinations. Through photoluminescence excitation (PLE) measurements excitation channels of the various bound excitons are obtained. In addition, the excitation channels for the free A-excitions are studied. These results yield new insight into the energy transfer processes. Finally, we present infrared (IR) transmission data indicating the presence of deep impurities which may trap carriers and also affect the bandgap luminescence.

HL 38.10 Wed 12:00 H17

Donator-Akzeptor-Komplexbildung in ZnO — •Muhammed Türker, Peter Reichert, Manfred Deicher, Herbert Wolf und Thomas Wichert — Technische Physik, Universität des Saarlandes, 66123 Saarbrücken

Nach wie vor bereitet im Gegensatz zur n-Dotierung die p-Dotierung von ZnO große Schwierigkeiten. Als Möglichkeit für eine verbesserte p-Dotierung werden nach theoretischen Überlegungen die Donator-Akzeptor-Kodotierung [1] oder die Cluster-Dotierung [2] vorgeschlagen. Dabei führt die Bildung von Donator-Akzeptor-Komplexen zur Steigerung der p-Leitfähigkeit. Experimentell wurde dieser Ansatz für die In-N-Kodotierung durch elektrische Messungen bestätigt [3]. Auf atomarer Ebene sind solche Defektkomplexe durch elektrische Feldgradienten (EFG) am Ort des Donators charakterisiert, die mit Hilfe der gestörten $\gamma\gamma$-Winkelkorrelation (PAC) und des radioaktiven Donators ^{111}In bestimmt werden können. Für verschiedene Verfahren der In-Akzeptor-Kodotierung (Implantation und/oder Diffusion) wurden neben dem EFG des ungestörten ZnO-Gitters ($\nu_{QGitter}$ = 31 MHz) durch weitere EFG charakterisierte Defekte beobachtet, die auf eine Bildung von In-N- und In-P-Komplexen hinweisen. Unter Berücksichtigung von druckabhängigen PAC-Messungen und ergänzenden Diffusionsprofilmessungen werden die Messergebnisse diskutiert.

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[1] T. Yamamoto *et al.*, Physica B **302-303** (2001) 155
[2] L.G. Wang *et al.*, Phys. Rev. Lett. **90** (2003) 256401
[3] L.L. Chen *et al.*, Appl. Phys. Lett **87** (2005) 252106

HL 38.11 Wed 12:15 H17

Electrical characterization of single-crystal ZnO grown by different techniques. — •Vladimir Kolkovsky, Leopold Wolff, Xi Zhang, and Joerg Weber — Technische Universität Dresden, 01062 Dresden

In the present study single-crystal ZnO grown by different techniques (hydrothermal technology, melting-grown crystals and crystals from the vapor phase) have been investigated with electrical measurements such as current-voltage (IV), capacitance-voltage (CV) and deep level transient spectroscopy (DLTS). Properties of Schottky contacts formed on ZnO grown with these techniques have been also analysed and compared. In DLTS studies dominant peaks appear in the range of 120-170 K in all materials studied. However, the properties of the DLTS lines are different and depend on the growth procedure of ZnO. The origin of these lines will be discussed in the present work.

HL 38.12 Wed 12:30 H17

A novel method to determine optical emission rates of defect-trapped electrons with high precision — •Martin Ellguth, Florian Schmidt, Matthias Schmidt, Holger v. Wenckstern, Rainer Pickenhain, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II

The properties of defects as the primary factor influencing the electrical behaviour of a semiconductor are one of the most important targets of semiconductor research, especially in novel materials like ZnO where the causes of unintended electrical behaviour in fabricated samples are often unknown. Existing publications on defects in ZnO report the activation energy and the carrier capture cross-section as well as occurence of defects in specially prepared samples. We extend this data set by providing photo cross-section spectra with the high accuracy necessary to determine meaningful values for the Franck-Condon parameter. A novel technique to reliably determine the emission rates of defect-trapped electrons excited by photon absorption ("optical" emission) is presented. It is similar to isothermal DLTS. Long transients (up to 1 hour) are digitally recorded while the sample is illuminated with monochromatic light and transformed into a rate spectrum. Varying the photon energy, the rates of optical emission processes can be determined from each spectrum to enable the calculation of the photo cross-section spectra with excellent precision. The thermal binding energy of a very deep defect not accessible in standard DLTS has been estimated from such a spectrum by applying a model from [1].

[1] A. Chantre, G. Vincent, D. Bois, Phys. Rev.˜B 23, 5335 (1981)

HL 38.13 Wed 12:45 H17

Temperature-dependent time-resolved photoluminescence on MgZnO — •Alexander Müller, Marko Stölzel, Christof Dietrich, Gabriele Benndorf, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

ZnO is a promising material for optoelectronic applications in the UV spectral range. By alloying it with MgO, the band gap of the resulting MgZnO can be increased, making it a suitable barrier layer for ZnO-based quantum wells. To investigate the dynamic carrier properties in this material, we have performed time-resolved photoluminescence (TRPL) measurements on PLD-grown $Mg_xZn_{1-x}O$ thin films with $x \leq 0.33$. Carrier thermalization and localization effects have been investigated by temperature-dependent TRPL measurements. At low temperatures, the excitons in this alloy are strongly localized. For samples with low Mg concentration, the spectrum is dominated by impurity-bound excitons exhibiting a fast decay. For large Mg contents, the excitons are mainly localized in randomly distributed alloy-potential minima, showing a slow, non-exponential decay process. With increasing temperatures, the decay time strongly decreases, indicating a transfer of the excitons to non-localized, free states. This explanation will be supported by Monte Carlo simulations.