HL 39: ZnO and Relatives II

Time: Tuesday 11:30–13:15 Location: EW 202

HL 39.1 Tue 11:30 EW 202

A DFT study of N impurities in ZnO nanoparticles — •Johann Gutjahr, Sung Sakong, and Peter Kratzer — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Duisburg, Germany

Zinc oxide nanostructures have attracted increasing interest due to their promising applications in electronic devices. ZnO is possibly ideally suited for blue/UV light-emitting diodes or laser diodes, once n- and p-doped ZnO can be produced reliably and reproducably. Nevertheless, p-type ZnO was obtained experimentally by N doping (Nature Materials **4**,42(2005)). We study N doping of nanoparticles (NP) because their properties can be tuned and they offer a simple way to produce ZnO material by e.g. sintering. In bulk ZnO, DFT calculations show the deep character of the N impurity on the O site because of the too high position of the charge transfer level $(0/-)$ in the band gap (APL **95**,252105(2009)).

As expected, the NP HOMO-LUMO gap is increased with decreasing NP size, but the N defect formation energy is found to be similar to bulk ZnO. Moreover, from the change of electron affinity we conclude the deepness of the N acceptor level. We also study different kinds of passivation and find that with H-passivation the adsorbate-induced states lie between VBM and acceptor level. Based on this, we explore the N acceptor level in thin ZnO-films as a model for the surface of a bigger particle to learn more about the influence of H-induced states.

HL 39.2 Tue 11:45 EW 202

Passivation of tungsten trioxide gated MISFETs based on ZnO channel material — •Anna Reinhardt, Michael Lorenz, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group

Recently, tungsten trioxide was reported to be an advantageous high-k gate oxide for transparent MISFETs with large on/off current ratios and low gate-voltage sweeps due to a high dielectric constant ($\epsilon_r \approx 70$)[1]. However, a slight hysteresis limiting the device switching speed occurs in the transfer characteristic.

The passivation of TFTs with lithographically processed SU-8 resist is very promising, providing a non-vacuum and low temperature process (max. 90 °C) compared to other deposition methods for passivation layers such as sputtering. We present our results on passivated tungsten oxide gated MISFETs deposited at room temperature on ZnO channel using pulsed-laser deposition. The electrical properties including on/off ratio, field-effect mobility and transfer characteristic are investigated by current-voltage measurements. In order to investigate the origin of the hysteresis and to study the distribution and density of defects quasi-static capacitance-voltage measurements as well as capacitance-voltage spectroscopy using different probing voltage frequencies were performed. Furthermore, time and temperature stability is compared to unpassivated devices.

[1] M. Lorenz *et al.*, Adv. Mater., doi: 10.1002/adma.201103087

HL 39.3 Tue 12:00 EW 202

Temperature dependent properties of ZnO/(Mg,Zn)O quantum wells with and without a distinct QCSE — •Marko Stölzel, Johannes Kupper, Matthias Brandt, Alexander Müller, Gabriele Benndorf, Michael Lorenz, and Marius Grundmann — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Confinement effects, the Stokes shift and the quantum-confined Stark effect (QCSE) determine the luminescence properties of polar ZnO/(Mg,Zn)O quantum wells (QWs). We present temperature dependent photoluminescence and optical transmission measurements to separate these effects and determine the origin of the luminescence.

Single QW structures have been prepared by pulsed laser deposition (PLD) on a-plane sapphire substrate exhibiting excitons with and without a distinct QCSE. The QCSE leads to a redshift of the QW luminescence maximum beneath the free exciton energy in ZnO as well as a change of the dynamics from a single exponential decay function to a non-exponential one, well described by a stretched exponential decay function. The internal electric field was evaluated to 0.66 MV/cm. Based on QWs without a distinct QCSE, the Stokes shift will be determined in dependence of well width and temperature.

The radiative decay time was found to increase linearly with temperature for both types of QWs indicating free exciton emission as the major recombination channel. With increasing temperature, the internal electric field is screened by free charge carriers, leading to a drop of the radiative decay time and reduction of the redshift above 50 K.

HL 39.4 Tue 12:15 EW 202

Electrical characterization of proton-irradiated MgZnO thin films — •Florian Schmidt[1], Matthias Schmidt[1], Holger von Wenckstern[1], Daniel Spemann[2], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — [2]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Nukleare Festkörperphysik, Linnéstraße 5, 04103 Leipzig

Zinc oxide (ZnO) is a semiconductor which is known for its high radiation hardness making the material suitable for space applications. Ternary MgZnO is an excellent material system for the fabrication of quantum well heterostructures and thus for potential application in exciton-related photonic devices. Whereas the influence of proton bombardment on the incorporation of defects in pure ZnO has been reported [1], no data are yet available regarding the exposure of MgZnO to protons. To study the effect of radiation, $Mg_{1-x}Zn_xO$ thin films with Mg contents of $0 \leq x \leq 2\%$ were irradiated by 2.25 MeV protons with fluences ranging from $1 \times 10^{13}\,cm^{-2}$ to $2 \times 10^{14}\,cm^{-2}$. The samples grown by pulsed-laser deposition were characterized by means of C-V measurements, deep level transient spectroscopy (DLTS) and Laplace DLTS. The proton irradiation generates a deep-level, labelled E4 in the literature, which has been tentatively assigned to the oxygen vacancy [1,2]. The generation rate of the defect in the MgZnO thin films was determined.

[1] F. D. Auret *et al.*, Appl. Phys. Lett., **79**(19), 3074 (2001).
[2] T. Frank *et al.*, Appl. Phys. A **88**, 141 (2007).

HL 39.5 Tue 12:30 EW 202

Raman spectra of ZnO and nitrogen doped ZnO – Tensor elements and additional modes — •Thomas Sander, Christian Reindl, Sebastian Eisermann, Elisabeth A. Zolnowski, Stefan Lautenschläger, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Gießen

Raman spectra of wurtzite ZnO have been studied intensively in the past. However, some unanswered questions still remain, like the Raman tensor elements, which have not been determined yet and are of fundamental physical interest. Furthermore, ZnO is a promising candidate for potential applications in optics and optoelectronics in the near UV region, if one overcomes the lack of reliable p-type doping. Nitrogen is an acceptor in ZnO. Incorporating N into ZnO leads to several additional modes in Raman spectra whose origins are still controversial.

Wurtzite bulk ZnO substrates and nitrogen doped ZnO thin films grown by CVD were studied by Raman spectroscopy. The phonon spectra were recorded in backscattering geometry at room temperature. The samples were rotated around the axis defined by the 532 nm, polarized excitation laser in different scattering geometries. The results allow one to determine the four tensor elements of ZnO and proof the fundamental selection rules. Furthermore, they will shed light on the origin of the controversially discussed additional Raman modes in the spectra caused by the nitrogen incorporation.

HL 39.6 Tue 12:45 EW 202

Hyperfeinwechselwirkung in ZnO unter uniaxialem Druck — •Rita Przewodnik und Reiner Vianden — Helmholtz-Institut für Strahlen und Kernphysik, 53115 Bonn, Deutschland

Untersucht werden Zinkoxid Einkristalle unter uniaxialer Belastung im Druckbereich von 0-300 MPa. Aufgrund der Wurtzitstruktur bildet sich ein zur c-Achse axialsymmetrischer, elektrischer Feldgradient (EFG) aus, dessen Betrag vom c/a Verhältnis der Kristallachsen abhängt. Das Verhältnis der Kristallachsen ändert sich im Belastungsfall, womit der EFG beeinflusst wird.

Die Änderung des EFG in Abhängigkeit von der externen Druckspannung wird mit der Methode der gestörten γ-γ-Winkelkorrelation (Perturbed Angular Correlation, PAC) bestimmt. Als Sonden werden

dazu ^{111}In-Ionen implantiert, die substitutionell auf Zinkplätzen ins Kristallgitter eingebaut werden. Die entstehenden Implantationsschäden werden vor der Messung ausgeheilt. Die Experimente zeigen in dem betrachteten Druckbereich eine lineare Zunahme des EFG bei uniaxialer Druckerhöhung in Richtung der c-Achse. Eine Druckerhöhung entlang der m-Achse führt zu einer linearen Abnahme bei zunehmender Asymmetrie des EFG.

HL 39.7 Tue 13:00 EW 202

Hydrostatic pressure dependence of the refractive index in ZnO and GaN — •Felix Käss[1,2], Juan Sebastian Reparaz[1,2], Gordon Callsen[2], Markus Raphael Wagner[2], Alejandro Rodolfo Goñi[1,3], Maria Isabel Alonso[1], Miquel Garriga[1], and Axel Hoffmann[2] — [1]Institut de Ciència de Materials de Barcelona-CSIC, Esfera UAB, 08193, Bellaterra, Spain — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, u o a 10623 Berlin, Germany — [3]ICREA, Passeig Lluís Companys 23, 08010 Barcelona, Spain

In this work we will present the hydrostatic pressure dependence of the real part of the refractive index in ZnO and GaN. By using a diamond anvil cell (DAC) combined with an optical transmission experiment we study the Fabry-Pérot interferences in the transparency region (approx. below 3.2 eV). A large series of interference peaks arising from the cavity-modes allow for the determination of the energy dependent refractive index. Many experimental complications which we found to be critical will be discussed in detail, leading to a detailed description of the optimum characteristics which are required for an ethalon to optically manifest in the DAC enviroment.