

## HL 97: ZnO

Time: Friday 9:30–12:30

Location: H16

HL 97.1 Fri 9:30 H16

**Controlled Growth of ZnO Nanowires from Thermal CVD - The Role of Carrier Gas Flow and Species Diffusion** — ●ANDREAS MENZEL<sup>1</sup>, RAYE GOLDBERG<sup>2</sup>, GUY BURSTHETIN<sup>2</sup>, VICTOR LUMELSKY<sup>2</sup>, KITTITAT SUBANNAJUI<sup>1</sup>, YESHAYAHU LIFSHITZ<sup>2</sup>, and MARGIT ZACHARIAS<sup>1</sup> — <sup>1</sup>Laboratory for Nanotechnology, IMTEK - Department of Microsystems Engineering, University of Freiburg, Freiburg, Germany — <sup>2</sup>Faculty of Materials Engineering and Russel Berrie Nanotechnology Institute, Technion Israel Institute of Technology, Haifa 32000, Israel

Nanowires (NWs) are promising materials for future electronics, optics and sensor device applications. Typically, ZnO NWs are grown in a tube furnace which includes that the respective material necessary for the desired NW materials is evaporated and transported toward a substrate. Hence evaporation efficiency, diffusion and gas flow are mandatory for a successful growth. When the transported species approaches the substrate nucleation, diffusion and growths occurs. A huge amount of work reports about growth of NWs by thermal CVD, however, the role and influence of growth parameters still remains unclear. Different parameters, geometries (diameters, inner and outer tube configurations etc.) as well as growth parameters (temperature, carrier gas and pressure) are reported, but cannot really be compared. We systematically studied and simulated the distribution of the growth species in such tube processes combined with growth experiments and evaluate their effects on the NW growth. Diffusion and convection can be tuned in a controlled way to achieve balanced steady growth conditions.

HL 97.2 Fri 9:45 H16

**Growth of ZnO nanowires for sensor applications** — ●MANFRED MADEL, FELIX SENF, TERESA BAUR, MARTIN DICKEL, SIMON BERKE, SEBASTIAN BAUER, INGO TISCHER, BENJAMIN NEUSCHL, UWE RÖDER, and KLAUS THONKE — Institut für Quantenmaterie / Gruppe Halbleiterphysik, Universität Ulm

ZnO nanowires with average diameter of 50 nm and length up to 10  $\mu\text{m}$  were grown by chemical vapour deposition and reveal suitability for sensor applications due to a large surface to volume ratio. Good crystal quality and excellent structural definition is shown by scanning electron microscopy, X-ray diffraction as well as by photo- and cathodoluminescence measurements. Photoconductivity measurements were performed either by direct contacting single pillars via a conductive atomic force microscope tip, or using interdigital structures, on which the wires were aligned by a dielectrophoresis method. The wires show a high sensitivity to light with a threshold for persistent photoconductivity of around 2.8 eV. Optical readout with a micro-PL setup shows a clear change of the signal intensity in different gas ambient atmospheres.

HL 97.3 Fri 10:00 H16

**Atomistic simulations of organic/ZnO hybrid nanowires** — ●ADRIEL DOMÍNGUEZ, SVEA GROSSE HOLTHAUS, ANDREIA DA ROSA, and THOMAS FRAUENHEIM — Bremen Center for Computational Materials Science, University of Bremen, Am Fallturm 1, 28359, Bremen, Germany

The understanding of the interaction of organic species with inorganic surfaces and nanostructures constitutes an important step in the development of semiconductor hybrid devices such as solar cells and biosensors. Density functional theory has been employed to investigate the atomic and electronic structure of ZnO nanowires modified with glycine and substituted methane molecules. We have identified -COOH, -NH<sub>2</sub>, -PO(OH)<sub>2</sub> and -SH as suitable anchoring groups for binding to the ZnO nanowires[1-3]. We have found three relevant mechanisms acting on the interface stabilisation: passivation of surface oxygen lone-pairs via dissociative chemisorption processes, electrostatic adsorbate-interaction involving Zn surface sites and hydrogen bonding involving adsorbates and oxygen surface sites. We will further discuss the role of water and hydroxyl groups on the adsorption mode and stabilisation of these functional groups[4].

References: [1] N. H. Moreira, A. L. da Rosa, Th. Frauenheim, Appl. Phys. Lett. 94, 193109 (2009). [2] N. H. Moreira, A. Dominguez, Th. Frauenheim, and A. L. da Rosa, Phys. Chem. Chem. Phys. 14, 15445 (2012). [3] X. Q. Shi, H. Xu, M. A. van Hove, N. H. Moreira, A.

L. da Rosa and Th. Frauenheim, Surf. Sci. 606,289 (2012). [4] A. Dominguez, S. grosse Holthaus, A. L da Rosa and Th. Frauenheim, to be submitted.

HL 97.4 Fri 10:15 H16

**Electrical and optical properties of room temperature deposited zinc tin oxide thin films and utilisation in all oxide amorphous heterodiodes** — ●PETER SCHLUPP, FRIEDRICH LEONARD SCHEIN, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN — Universität Leipzig, Germany

To provide cost-efficient and homogeneous oxide thin films it is desirable to use amorphous materials which can be deposited at room temperature (RT). Zinc tin oxide (ZTO) is a promising n-type channel material and is in contrast to the well explored amorphous transparent semiconducting oxide GaInZnO indium-free and with that less expensive. We present electrical and optical properties of RT-deposited ZTO thin films. The films were fabricated via pulsed laser deposition on glass substrates from an 1:2 ZnO : SnO<sub>2</sub> target. The background gas (O<sub>2</sub>, N<sub>2</sub> or Ar) pressure was varied systematically from  $3 \times 10^{-4}$  mbar to 0.1 mbar. The resistivity can be tuned over several orders of magnitude, from insulating for high and low pressures down to  $1.7 \times 10^{-4} \Omega\text{m}$  for intermediate pressure. All films investigated are X-ray amorphous. In the visible spectral range (400-800nm wavelength) the optical transmission is about  $T_{\text{vis}} = 40 - 85\%$ , depending on the fabrication partial pressure. Optimized ZTO layers were used to fabricate an all amorphous pin heterodiode consisting of ZnCo<sub>2</sub>O<sub>4</sub> and ZTO. The rectification of the device is about  $6 \times 10^3$  at  $U = \pm 1\text{V}$  at RT. Further, temperature-dependent I-U characteristics will be discussed.

HL 97.5 Fri 10:30 H16

**The role of the surface in resonance Raman scattering in ZnO and other wurtzites** — ●CHRISTIAN KRANERT, RÜDIGER SCHMIDT-GRUND, and MARIUS GRUNDMANN — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Leipzig, Germany

We apply the double resonance model of R. M. Martin [1] to the resonance Raman scattering by longitudinal optical (LO) phonons in ZnO, excited well above the band gap ( $\lambda = 325\text{nm}$ ). By extending this model with an elastic scattering process at the surface, we provide an improved understanding of the physical background and the spectral properties of the 1LO line. The consideration of the surface-related process, additionally to the well-established elastic scattering by point defects, is essential to conclusively explain several experimental findings. Particularly, the dependence of the peak position on the orientation of the excited surface cannot be understood otherwise. It was previously attributed to the varying wave vectors of the incident and scattered light in the literature which we will disprove theoretically and experimentally. We will present similar experimental results for other wurtzites (GaN, InN, CdS) which show the general validity of this extended model.

[1] R. M. Martin, Phys. Rev. B 10, 2620 (1974)

**Coffee break**

HL 97.6 Fri 11:00 H16

**Raman scattering of H<sub>2</sub> in ZnO** — ●SANDRO G. KOCH, EDWARD V. LAVROV, and JÖRG WEBER — Technische Universität Dresden, 01062 Dresden, Germany

ZnO single crystals thermally treated in a H<sub>2</sub>, D<sub>2</sub>, or H<sub>2</sub> + D<sub>2</sub> ambient at 800–1000 °C are studied by Raman scattering. Directly after the treatment most hydrogen forms shallow donors at the bond-centered site. Subsequently, interstitial hydrogen migrates through the lattice and forms electrically inactive H<sub>2</sub>. The formation process, thermal stability, interaction with the phonon spectrum, position of the molecule in the host lattice, as well as the ortho-para conversion rate are addressed in this study. It is shown that H<sub>2</sub> in ZnO is almost a free rotator, which is stable in the temperature range 300–600 °C. Arguments are presented that the molecule occupies an interstitial lattice site. It is also shown that at elevated temperatures the para species is absent in Raman spectra, which is explained by thermally activated excitation of the molecule from the  $J = 0$  to the  $J = 2$  rotational state and phonon broadening of the spectral line associated with  $J = 2$ .

HL 97.7 Fri 11:15 H16

**PLE of ZnO/(Zn,Mg)O quantum well structures on sapphire** — ●AXEL RÖMER, MARKUS WAGNER, CHRISTIAN NENSTIEL, GORDON CALLEN, MAX BÜGLER, and AXEL HOFFMANN — Technische Universität, Berlin, Germany

In this work ZnO/(Zn,Mn)O multi-quantum-well structures are investigated. Through optical characterisation methods we examined the recombination dynamics and luminescence of different samples. Variation of crystal orientation and quantum well thickness in different samples leads to investigation of the dependence of the recombination behaviour of the material system on the quantum well structure and as well of the orientation of the crystal of the samples. Through the measurements it was cleared out which processes take part in the luminescence, whereas the main luminescence of the quantum well was focused on. Further more the samples were investigated with photoluminescence excitation spectroscopy (PLE). Not only the different processes could be observed, it was also possible to examine the excitation channels of those processes. With additional variation of polarisation and temperature through the PLE measurements it is possible to see more interesting details in the recombination dynamics until up to 4eV and get further information about those processes.

HL 97.8 Fri 11:30 H16

**Ion-induced luminescence of radiation defects in ZnO** — ●RONALD STÜBNER<sup>1</sup>, JÖRG WEBER<sup>1</sup>, DANIEL SEVERIN<sup>2</sup>, and MARKUS BENDER<sup>2</sup> — <sup>1</sup>Technische Universität Dresden, Germany — <sup>2</sup>Gesellschaft für Schwerionenforschung, Darmstadt, Germany

A study of ion-induced luminescence of ZnO at low temperatures is presented. Based on the distinct difference between photo- and ion-induced luminescence spectra, it is concluded that the ion-induced luminescence results from excitonic recombinations at irradiation induced native defects. By comparison of the properties of the observed luminescence features with the data known from the literature, these features are assigned to the so far unidentified  $I_{10}$  defect (3.353 eV). The zinc interstitial is suggested as the possible origin of the  $I_{10}$  line.

HL 97.9 Fri 11:45 H16

**Irradiation studies on differently orientated ZnO thin films** — ●FLORIAN SCHMIDT<sup>1</sup>, HOLGER VON WENCKSTERN<sup>1</sup>, STEFAN MÜLLER<sup>1</sup>, DANIEL SPEMANN<sup>2</sup>, and MARIUS GRUNDMANN<sup>1</sup> — <sup>1</sup>Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — <sup>2</sup>Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Nukleare Festkörperphysik, Linnéstraße 5, 04103 Leipzig

Zinc oxide (ZnO) is a wide-bandgap semiconductor which is known for its high radiation hardness. The influence of proton bombardment on the incorporation of defects in  $\pm c$ -oriented ZnO bulk crystals [1] and thin films [2] has been reported previously, no data are available regarding the exposure of differently orientated ZnO to protons. The orientation of the thin films is predetermined by the orientation of the sapphire substrates. We grew  $c$ -,  $a$ -, and  $m$ -plane ZnO thin films on  $a$ -,  $r$ -,  $m$ -plane sapphire, respectively, by pulsed laser deposition. To study the effect of radiation, the films were irradiated by 2.25 MeV protons with fluences ranging from  $1 \times 10^{13} \text{ cm}^{-2}$  to  $2 \times 10^{14} \text{ cm}^{-2}$

and characterized by means of  $C$ - $V$  measurements, deep level transient spectroscopy (DLTS) and Laplace DLTS.

Proton irradiation generates a deep-level, labelled E4 in the literature [3], which was tentatively assigned to the oxygen vacancy. The generation rate of this defect in the ZnO thin films was determined.

- [1] F. D. Auret *et al.*, Appl. Phys. Lett., **79**(19), 3074 (2001).
- [2] F. Schmidt *et al.*, Appl. Phys. Lett. **101**, 012103 (2012).
- [3] T. Frank *et al.*, Appl. Phys. A **88**, 141 (2007).

HL 97.10 Fri 12:00 H16

**Iron-induced gap states in ZnO thin films** — ●RAINER PICKENHAIN<sup>1</sup>, FLORIAN SCHMIDT<sup>1</sup>, SEBASTIAN GEBURT<sup>2</sup>, CARSTEN RÖNNING<sup>2</sup>, HOLGER VON WENCKSTERN<sup>1</sup>, and MARIUS GRUNDMANN<sup>1</sup> — <sup>1</sup>Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — <sup>2</sup>Institute for Solid State Physics, University of Jena, Helmholtzweg 3, D-07743 Jena

States of the transition metal iron within the bandgap of ZnO are not satisfyingly understood yet. Experimental evidence concerning internal transitions at about 1.8 eV [1] and 0.4 eV [2], respectively, of iron in  $\text{Fe}^{3+}$  and  $\text{Fe}^{2+}$  configuration exist. A concise experimental determination of the energetic position of these states within the bandgap was, however, not accomplished. In this study we present results on a ZnO thin film that was iron-implanted with a total fluence of  $2 \times 10^{11} \text{ ions/cm}^2$ . Due to the implantation/annealing process the net doping density decreased from  $8 \times 10^{16} \text{ cm}^{-3}$  to  $1 \times 10^{16} \text{ cm}^{-3}$ . By employing low-rate optical deep level transient spectroscopy (LR-ODLTS) we were able to detect two formerly not discovered states in the ZnO bandgap which we attribute to the incorporation of iron on zinc lattice site. These states lie at room temperature about 150 meV over the ZnO valenceband and 2200 meV below the ZnO conduction band minimum. Temperature-dependent measurements reveal that transition energies of these states increase similar to the ZnO bandgap down to 4 K.

- [1] R. Heitz *et al.*, Phys. Rev. B, **45**, 8977 (1992).
- [2] E. Malguth *et al.*, Phys. Stat. Sol. (b) **245**, 455 (2008).

HL 97.11 Fri 12:15 H16

**Synchrotron based spectroscopic ellipsometry of MgZnO** — ●MACIEJ D. NEUMANN<sup>1</sup>, CHRISTOPH COBET<sup>2</sup>, MARTIN FENEBERG<sup>3</sup>, RÜDIGER GOLDHAHN<sup>3</sup>, JEAN-MICHEL CHAUVEAU<sup>4</sup>, and NORBERT ESSER<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., 12489 Berlin, Germany — <sup>2</sup>Johannes Kepler Universität Linz, 4040 Linz, Austria — <sup>3</sup>Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany — <sup>4</sup>Centre de Recherche sur l'Hétéro-Epitaxie et ses Applications, 06565 Sophia Antipolis, France

Using a newly developed synchrotron VUV ellipsometer allowing variable angle of incidence studies, non-polar MBE grown MgZnO samples with Mg contents up to 45% were investigated in the photon energy range from 2 to 25 eV. For the first time, both the parallel and perpendicular components of the complex dielectric tensor are presented. The strength of optical anisotropy above 10 eV decreases continuously with increasing Mg content. It suggests that the optical transitions in this range are strongly related to the Zn-3d levels. The results are in remarkable agreement to novel ab-initio calculations.