

HL 38: Zinc Oxide

Time: Tuesday 9:30–11:15

Location: POT 06

HL 38.1 Tue 9:30 POT 06

Al-doped ZnO nanowires grown by PLD — ●ALEXANDER SHKURMANOV, CHRIS STURM, HOLGER HOCHMUTH, and MARIUS GRUNDMANN — Universität Leipzig, Inst. for Exp. Phys. II, Linéstr. 5, 04103 Leipzig, Germany

ZnO nanowires (NWs) attract a lot of interest and can be used as building blocks for different devices e.g. light emitters, resonators and sensors. At the same time, doping of the ZnO NWs by Al leads to increase of their conductivity [1], luminescence intensity [2], and optical transmission [3] in comparison with undoped ZnO. This makes doped ZnO NWs promising for a wide range of applications.

Here we present the growth of Al doped ZnO NWs on ZnO seed layers by pulsed laser deposition (PLD). We demonstrate that the choice of the seed layer as well as a growth temperature determine the shape of the NWs and allow to vary diameter of the NWs diameter from 550 nm to less than 7 nm. Furthermore, by comparing the NW growth of undoped ZnO wires on the same kind of the seed layers allows deeper insight into the growth mechanism of the ZnO wires.

[1] G. Zimmermann et al., Phys. Status Solidi RRL 4, 3-4 2010

[2] C.-L. Hsu et al., RSC Adv., 4, 2980, 2014

[3] C. M. Garcia et al., Advances in Materials Physics and Chemistry, 2, 56, 2012

HL 38.2 Tue 9:45 POT 06

Unambiguous identification of Sn₃O₄ using Raman spectroscopy and ab initio calculations — ●CHRISTIAN T. REINDL¹, MARTIN BECKER¹, BIANCA K. EIFERT², MARCEL GIAR², LILAN ZHENG³, ANGELIKA POLITY¹, YUNBIN HE³, CHRISTIAN HEILIGER², and PETER J. KLAR¹ — ¹I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — ²Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — ³Faculty of Materials Science and Engineering, Hubei University, Wuhan 430062, China

A lot is known about the two stable tin oxides SnO and SnO₂. Both phases have been intensively investigated and are widely used in applications such as transparent conducting oxides, gas sensors, and lithium ion batteries. Over the last century many attempts have failed to identify the metastable oxide occurring at an intermediate Sn:O stoichiometry. Using Raman spectroscopy as the experimental backbone and ab initio density functional theory (DFT) calculations we are able to distinguish different candidates and finally identify the intermediate phase as Sn₃O₄. The samples evaluated are of different origin. One kind was grown utilizing ion beam sputter deposition (IBSD) directly, whereas the second kind was first ion beam sputtered as SnO and annealed to form the intermediate phase. The third kind was a SnO layer produced by pulsed laser deposition which was oxidized to the intermediate phase afterwards. All three variants show none or only slight traces of SnO or SnO₂, respectively and are in excellent agreement with the calculated Sn₃O₄ spectra.

HL 38.3 Tue 10:00 POT 06

Polymer passivated zinc oxide thin film transistors — ●TORSTEN BALSTER, JONAS KÖHLING, MARLIS ORTEL, and VEIT WAGNER — Department of Physics and Earth Sciences, Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Thin film transistors with ZnO as active layer were prepared by pulsed spray pyrolysis method, in order to investigate the passivation of surface trap states. These states are known to have significant influence on mobility, hysteresis and stability of transistors. Promising candidates for the passivation are polymer classes containing an oxygen with free electron pairs, which can coordinate with Zn-atoms at the surface.

After the pulsed spray pyrolysis deposition of the ZnO films, poly methyl methacrylate, which has a carbonyl group in the monomer, was spin-coated from solution onto the TFT and annealed afterwards. After this treatment, no hysteresis and only a minor onset voltage variation during bias stress could be observed. However, the onset was shifted to lower values in comparison to the untreated surface. Furthermore, the influence of the molecular chain length and the solvent on the electronic properties will be discussed.

Coffee Break

HL 38.4 Tue 10:30 POT 06

Defects and defect complexes in zinc oxide revisited: Self-consistent hybrid functional calculations — ●DANIEL FRITSCH¹, BENJAMIN MORGAN¹, and ARON WALSH^{1,2} — ¹Department of Chemistry, University of Bath, BA2 7AY Bath, UK — ²Department of Materials, Imperial College London, SW7 2AZ London, UK

Zinc oxide exhibits *n*-type conductivity, arising from intrinsic defects and hydrogen impurities, and this can be enhanced by aliovalent doping with group-III elements. Al-doping of ZnO is a particular example of this doping strategy with great potential for use in future technologies and devices. The effect of Al-doping depends on the delicate interplay between intrinsic point defects (V_{Zn} , V_O , Zn_i , O_i) and substituted Al (Al_{Zn}). In particular, our understanding of possible complex formation, such as the aluminum–zinc-vacancy complex ($Al_{Zn}-V_{Zn}$), is far from complete and requires further detailed investigations.

Most recent density functional theory calculations of ZnO doping have used hybrid functionals, which introduce a fraction of Hartree-Fock exchange into available exchange-correlation potentials based on intuition or experimental calibration. A recent self-consistent hybrid functional [1] offers a new approach for parameter-free hybrid functional investigations and removes this level of empiricism. Having used this new self-consistent hybrid method, we will present calculated results for bulk ZnO, its intrinsic defects, and the important $Al_{Zn}-V_{Zn}$ defect complex, and compare them to available experimental and theoretical data.

[1] J. H. Skone *et al.*, Phys. Rev. B 89, 195112 (2014).

HL 38.5 Tue 10:45 POT 06

Second-Harmonic Generation in ZnO/(Zn,Mg)O Multiple Quantum Wells — ●JOHANNES MUND¹, DMITRI R. YAKOVLEV¹, SERGEY SADOFEV², CEDRIK MEIER³, and MANFRED BAYER¹ — ¹Experimentelle Physik 2, Technische Universität Dortmund, Germany — ²Institut für Physik, AG Photonik, Humboldt-Universität zu Berlin, Germany — ³Department Physik, Nanophotonik & Nanomaterialien, Universität Paderborn, Germany

Non-linear optical properties of ZnO/Zn_{0.9}Mg_{0.1}O multiple quantum wells with well width varied from 1.8 to 10 nm are studied by second-harmonic generation (SHG).

We succeed to detect the 1S quantum well exciton and show qualitatively the quantum confinement of this state in narrow QW as well as the quantum confined stark effect in broader QW. A comparison to spectra of ZnO bulk material and a pure ZnMgO layer confirms that the observed resonance has its origin in the MQW structure. SHG spectra are compared with photoluminescence and reflectivity spectra to identify exciton transitions. Also SHG rotational diagrams are measured and relative values of components of the non-linear susceptibility tensor are evaluated.

HL 38.6 Tue 11:00 POT 06

Microdisks coupled with Waveguides of II/VI quantum well heterostructures — ●GESA SCHMIDT, TORSTEN RIEGER, DETLEV GRÜTZMACHER, and ALEXANDER PAWLIS — PGI-9 and JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Waveguides and microdisks were fabricated from II/VI quantum wells (QWs) grown by molecular beam epitaxy on GaAs substrates. They provide suitable components for integrated-optical devices in the blue/green spectrum. Additionally, doping of the QWs with fluorine allows modern devices such as low-threshold lasers and single photon sources and their integration. To this end, the introduction of an Al₂O₃ interlayer, fabricated by selective post-growth oxidation of an AlAs buffer between the GaAs and the II/VI heterostructure, provides improved waveguiding and reduced photon leakage. Al₂O₃ is optically transparent for the emission from the QWs and has considerably smaller refractive index compared to the II/VI material.

We present optical properties and photon-guiding characteristics of microdisk cavities with adjacent waveguide membranes. The analysis of spatial-resolved μ -photoluminescence measurements along the waveguide demonstrates the photon transfer between microdisk and waveguide. Moreover, we observed lasing at specific whispering gallery modes of our microdisks, which denote efficient photon guiding along the waveguide. Our findings demonstrate functional operation of microdisk-waveguide couplers based on ZnSe/(Zn,Mg)Se QW structures and their potential for larger scale integrated-optical systems in the blue/green spectral range.