HL 48: ZnO: Preparation and characterization II

Time: Thursday 9:30–10:30 Location: ER 164

HL 48.1 Thu 9:30 ER 164

Characterization of Mn doped ZnO Nanopowder — •Eva Schlenker[1], Andrey Bakin[1], Herbert Schmid[2], Werner Mader[2], Heiko Bremers[3], Andreas Hangleiter[3], Mohamed Al-Suleiman[1], Hergo-Heinrich Wehmann[1], and Andreas Waag[1] — [1]Institute of Semiconductor Technology, TU Braunschweig, 38106 Braunschweig — [2]Institute for Inorganic Chemistry, University of Bonn, 53117 Bonn — [3]Institute of Applied Physics , TU Braunschweig, 38106 Braunschweig

In the quest of materials for spintronic applications, diluted magnetic semiconductors recently attracted much attention. The main challenge is finding a ferromagnetic material with Curie temperature Tc $>$ 300 K whose magnetic properties can be controlled electrically. The interest was particularly focused on Zn(TM)O since theoretical calculations predict that ZnO containing Mn could exhibit ferromagnetism with Tc above room temperature. In the present study, the structural and magnetic properties of Mn doped ZnO nanopowder are investigated and compared to undoped ZnO crystals. Doping of ZnO with Mn results in increased lattice constants as revealed by XRD. However, an inhomogeneous distribution of the Mn dopants within the nanopowder was revealed by energy-dispersive X-ray and electron energy-loss spectroscopy. Magnetic properties are investigated by means of SQUID measurements on aggregates of powder particles as well as by MFM to study the behavior of single grains. The MFM image differs significantly from the topography as imaged by AFM and suggests the existence of long-ranging magnetic signals emerging from the sample.

HL 48.2 Thu 9:45 ER 164

As-Dotierung von homoepitaktisch abgeschiedenen ZnO-Schichten — •Sören Heinze, Andre Krtschil, Jürgen Bläsing, Hartmut Witte, Armin Dadgar, Frank Bertram, Peter Veit, Jürgen Christen und Alois Krost — Otto-von-Guericke-Universität Magdeburg, Fakultät für Naturwissenschaften, Institut für Experimentelle Physik

Zahlreiche Arbeitsgruppen konnten mittlerweile Erfolge bei der Homoepitaxie von ZnO auf thermisch vorbehandelten Substraten erzielen. Uns gelang dabei erstmals die homoepitaktische Abscheidung in einem 2-dimensionalen Wachstumsmodus, wie in Referenz [1] berichtet. Die Schichten zeigen dabei nicht nur exzellente morphologische sondern auch ausgezeichnete Lumineszenzeigenschaften hinsichtlich Homogenität der Wellenlänge und Intensität des emittierten Lichts, was an Hand von Kathodolumineszenzuntersuchngen gezeigt wurde. Desweiteren wurde mittels TEM-Untersuchungen die mikroskopische Ursache der Oszillationen in θ-2θ-XRD-Messungen welche von verschiedenen Autoren (z.B. in Referenz [2]) berichtet wurden aufgeklärt. Außerdem werden erste Ergebnisse zur As-Dotierung homoepitaktisch gewachsener Schichten präsentiert.

[1] S. Heinze et al. "Homoepitaxial growth of ZnO by metalorganic vapor phase epitaxy in two-dimensional growth mode", Journal of Crystal Growth 308, 170 (2007)

[2] D.J. Rogers et al. "ZnO homoepitaxy on the O polar face of hydrothermal and melt-grown substrates by pulsed laser deposition", Appl. Phys. A 88, (2007)

HL 48.3 Thu 10:00 ER 164

DFT/DFTB simulations of ZnO in bulk, surfaces, and nanostructures — •Christian Fisker — Dept. of Physics and Nanotechnology, Aalborg University, Denmark

As a large band gap semiconductor with the ability to form many different nanostructures, ZnO has gained a lot of interest in the scientific community. Numerical modelling using Density Functional Theory (DFT) has proven more difficult, as the complexity of the Zn d-orbitals greatly limits the size of the modelled system. A much more scalable treatment can be attained using Density Functional based Tight Binding (DFTB).

DFTB parameters for zinc oxide are presented in a manner that both the band gap and crystal structure of bulk ZnO are well reproduced. Surface geometry optimisations are tested against DFT calculations with good results, and the model is applied to calculating geometries and electronic properties of larger systems including nanowires.

HL 48.4 Thu 10:15 ER 164

ZnO:Mn^x valence configuration from the perspective of density functional theory — •Marc Andy Gluba and N. H. Nickel — Hahn-Meitner-Institut Berlin GmbH, Abt. Silizium Photovoltaik (SE1), Kekuléstraße 5, D-12489 Berlin, Germany

Zinc oxide (ZnO) doped with transition metal (TM) ions has attracted considerable interest because of its potential application as a base-material for spintronic devices. According to theoretical predictions by Dietl *et al.* manganese doped into ZnO should preserve its ferromagnetic order up to room temperature[1]. However, the experimental realization of dilute ferromagnetic ZnO is still challenging.

It is widely accepted that TM ions, when incorporated into the ZnO lattice, are isovalent with the zinc ions they substitute for. Thus, Mn in ZnO is commonly present in the divalent charge state for perceptibly high concentrations above 10^{19}cm^{-3}. However, recent electron paramagnetic resonance (EPR) experiments on ZnO with Mn traces of concentrations as low as 10^{14}cm^{-3} suggest that the Mn charge state can deviate from the divalent configuration[2]. In order to elucidate stable valence configurations of Mn and their respective transition levels bandstructure calculations have been performed in the framework of density functional theory (DFT). The impact of additional on-site coulomb interaction within the local spin density approach (LSDA+U) will be discussed.

[1] T. Dietl *et al.*, Science **287**, 1019 (2000)

[2] M. A. Gluba *et al.*, Superlattices and Microstructures (*in press*)