HL 83: Focus Session: Oxide semiconductors II (DS with HL)

Time: Thursday 15:00–19:00 Location: H 2032

Invited Talk HL 83.1 Thu 15:00 H 2032

Optical properties and band structure of transparent semiconducting oxides — •Rüdiger Goldhahn — Otto-von-Guericke-Universität Magedeburg, Institut für Experimentelle Physik

Semiconducting metal oxides such as cubic In_2O_3 and rutile SnO_2 have attracted much interest in recent years. High-quality bulk crystals and single-crystalline heteroepitaxial films, covering a wide range of electron concentrations, became available allowing the determination of intrinsic optical properties as well as related fundamental band-structure parameters. This talk summarizes recent achievements.

Spectroscopic ellipsometry from the infrared (IR) into the vacuum-ultraviolet (VUV) spectral region is applied for determining the components of the dielectric tensor. The analysis of the IR dielectric function yields the phonon frequencies and the coupled phonon-plasmon modes from which electron effective mass as a function of carrier density (nonparabolicity of the conduction band) is obtained. Many-body effects such as exciton screening, band-gap renormalization, and band filling have a strong impact on the behavior around the fundamental band gaps, a quantitative description of these properties will be presented. Finally, synchrotron-based studies in VUV provide the transition energies related to critical points of the band structure.

HL 83.2 Thu 15:30 H 2032

Optical and Magneto-Optical Investigation of Spinel Oxide Thin Films — •Vitaly Zviagin[1], Peter Richter[2], Christian Kranert[1], Tammo Böntgen[1], Michael Lorenz[1], Dietrich R.T. Zahn[2], Georgeta Salvan[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Technische Universtät Chemnitz, Semiconductor Physics, Reichenheiner Str. 70, Germany

We present a (magneto-) optical and structural investigation of Co_3O_4, $ZnFe_2O_4$, $CoFe_2O_4$, $ZnCo_2O_4$ and Fe_3O_4 spinel oxides grown at different temperatures on MgO (100) and $MgAl_2O_4$ (100) substrates by pulsed laser deposition. The optical properties were determined by spectroscopic ellipsometry in the spectral range from 0.5 eV to 8.5 eV and at temperatures from 10 K to 300 K. The magneto-optical response was measured in the range from 1.5 ev to 5.5 eV at room temperature and with an applied magnetic field of 1.7 T. A parametric model for the dielectric function, consisting of Gaussian and Lorenzian functions located at the optical transition energies, as well as the off-diagonal elements of the dielectric tensor were obtained. The magneto-optical response depends markedly on the crystal quality thus indicating the occurrence of mixtures of normal and inverse spinel structures. The study of (magneto-) optical properties is accompanied by structural analysis of the thin films using Raman spectroscopy, atomic force microscopy, and X-ray diffraction.

HL 83.3 Thu 15:45 H 2032

Spectroscopic signatures of dinitrogen in Cu_2O:N thin films — •Julian Benz, Philipp Hering, Benedikt Kramm, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

Cuprous oxide (Cu_2O) is an intrinsically p-type semiconductor with a band gap of 2.1 eV. By doping with nitrogen it is possible to increase the hole density significantly. Thin films of Cu_2O:N were prepared by reactive RF sputtering, providing N_2 gas as dopant in the plasma. Raman spectra of the N-doped samples exhibit additional signals in the region of 2200 cm^{-1} to 2300 cm^{-1} Raman shift, which scale with the nitrogen content. We assume that these signals can be assigned to the vibration of dinitrogen molecules bound at different sites inside the bulk and at the surface. To support our assumption, the influence of oxygen flow during growth, as well as growth and annealing temperature are investigated.

HL 83.4 Thu 16:00 H 2032

Structural properties and phonon modes of $(Al_xGa_{1-x})_2O_3$ — •Christian Kranert, Marcus Jenderka, Jörg Lenzner, Michael Lorenz, Holger von Wenckstern, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Leipzig, Germany

We present a combined X-ray diffraction and Raman scattering study on a 2-inch diameter thin film with a continuous composition spread (CCS) [1] in comparison to bulk-like ceramic samples. For the composition range for which the ceramic materials exclusively exhibit the β-modification, we obtained their individual lattice parameters as a function of the composition. These comply with Vegard's rule. We further investigated these samples by Raman spectroscopy. The obtained phonon energy dependencies on the composition in the β-phase are found to be linear as well.

The CCS approach for the thin films allows us to determine its properties for virtually any composition within the composition range of the sample. The comparison to the ceramic samples shows a reduced out-of-plane lattice parameter for the thin films. Despite that, the phonon energies show a good agreement to the bulk values.

The material β-Ga_2O_3 is of interest for deep UV optoelectronics. Alloying with Al_2O_3 increases its band gap, which makes the alloy $(Al,Ga)_2O_3$ suitable for an application in Ga_2O_3-based heterostructures or as barrier material for Ga_2O_3 quantum wells.

[1] H. von Wenckstern et al., CrystEngComm **15**, 10020 (2013)

HL 83.5 Thu 16:15 H 2032

Angle dependent Raman investigations of the different phases of Sn_xO_y — •Christian T. Reindl, Martin Becker, Bruno K. Meyer, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

The two widely known tin oxide phases SnO_2 and SnO are easily distinguished by examining their Raman spectra. Such Raman spectra contain information about the crystal structure and orientation as well as its quality, impurities, etc. Ion beam sputtered samples of SnO_2 and SnO with well-defined orientations are investigated using rotational Raman spectroscopy, a technique where the sample is rotated in plane with respect to the incident laser polarization. The intensity of the scattered light is analyzed for different polarizations with respect to the incident light. The data obtained is used to confirm the assignments of Raman modes appearing in the spectra of SnO_2 and SnO and to determine the values of the corresponding Raman tensor elements. Samples grown in the regime between the formation of these two phases yield completely different Raman spectra implies the formation of a third tin oxide phase in this intermediate regime. We present first identification of the Raman modes of this additional Sn_xO_y phase. Furthermore, naturally grown crystals are investigated and compared to the samples grown by ion beam sputtering and chemical vapor deposition.

15 min. break.

Invited Talk HL 83.6 Thu 16:45 H 2032

Thermodynamic stability and electronic structure of TCO surfaces: A computational approach — •Karsten Albe, Peter Agoston, Manuel Diehm, and Arno Fey — TU Darmstadt, FB 11, Fachgebiet Materialmodellierung, Jovanka-Bontschits-Str. 2, 64287 Darmstadt

A detailed understanding of the surface properties of transparent electrodes is a prerequisite for optimizing optoelectronic devices. In this contribution the thermodynamic stability and electronic properties of several experimentally observed low-index surfaces of bcc indium oxide (In2O3) and tin oxide (SnO2) are discussed based on results obtained by electronic structure calculations within density-functional theory. The influence of hydrogen, organic surfacants, n-type dopants (Sn), as well as the in-plane lattice strain are studied and compared to results of STM-studies on single crystalline samples. The computed data are also contrasted with results from photoelectron spectrocscopy on magetron-sputtered layers.

HL 83.7 Thu 17:15 H 2032

Defect studies on In_2O_3 thin films grown by pulsed laser deposition — •Florian Schmidt, Manuel R. Lindel, Daniel Splith, Stefan Müller, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

In_2O_3 is a promising oxide semiconducting material for applications in transparent electronics. Highly tin-doped In_2O_3 for instance is already

commercially exploited as transparent conducting electrode. However, less is known on the defect structure of the host material. The fabrication of rectifying Schottky contacts on In_2O_3 was reported recently [1] and opens up the possibility to apply space-charge spectroscopic methods, such as thermal admittanz spectroscopy (TAS) or deep-level transient spectroscopy (DLTS).

We investigated point defects in both undoped In_2O_3 and compensated In_2O_3:Mg thin films by means of TAS and DLTS. While a defect level with a thermal activation energy E_t of approximately 200 meV and an apparent capture cross-section σ_n of about 10^{-16} cm^2 was found both materials another deep defect with $E_t \approx 90$ meV and $\sigma_n \approx 5 \times 10^{-18}$ cm^2 was exclusively found in the Mg-doped sample.

[1] H. von Wenckstern *et al.*, APL Materials **2**, 046104 (2014).

HL 83.8 Thu 17:30 H 2032

Lattice dynamics of Copper-Oxide phases from ab initio calculations — •Marcel Giar, Thomas Sander, Markus Heinemann, Christian T. Reindl, Bianca Eifert, Peter J. Klar, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Lattice dynamic properties the three copper oxide phases Cu_2O, Cu_4O_3, and CuO are investigated employing DFT calculations using the VASP code. Phonon bandstructure and density of states for all three phases are derived from a supercell small displacement method. The splitting of the LO and TO modes at the Γ point is obtained by properly taking into account the non–analytical contributions to the dynamical matrix in the limit $\mathbf{q} \to 0$. We also examine Raman properties by calculating Raman susceptibilities and derived Raman spectra. Special attention is paid to the role of defects such as simple Cu vacancies (V_{Cu}) and Cu split vacancies (V_{Cu}^{Split}) in the Raman spectrum of Cu_2O.[1] Further, we present calculations on the low–frequency dielectric tensor from which also IR data can be derived.

[1] T. Sander, C. T. Reindl, M. Giar, B. Eifert, M. Heinemann, C. Heiliger, and P. J. Klar, Phys. Rev. B 90, 045203 (2014)

HL 83.9 Thu 17:45 H 2032

Determination of subgap states in oxides: a challenge for DFT functionals — Wolfgang Körner[1], •Daniel F. Urban[1], David Munoz Ramo[2], Paul D. Bristowe[2], and Christian Elsässer[1,3] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany — [2]Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom — [3]Institute for Applied Materials, Karlsruhe Institute of Technology

We present a density-functional-theory analysis of crystalline and amorphous Zn- and Sn-based oxide systems which focuses on the electronic defect-states within the band gap [1]. A comparison of these electronic levels reveals that the hybrid DFT exchange-correlation functionals PBE0, HSE06 or B3LYP agree with a self-interaction corrected local-density approximation (SIC-LDA) functional on occupied defect levels when similar treatments of the self-interaction are considered. However, for unoccupied levels the hybrid functionals and the SIC approach lead to very different predictions. We show that a prerequisite for the determination of the energetic position of subgap states in these oxides is that a functional needs to predict correctly the electronic band structure over a wide energy range and not just close to the band gap. We conclude that for accurate defect levels an adequate treatment of the self interaction problem is required especially in the presence of nearby metal-metal interactions.

[1] W. Körner, D. F. Urban, D. Munoz Ramo, P. D. Bristowe, C. Elsässer, Phys. Rev. B 90, 195142 (2014)

Invited Talk HL 83.10 Thu 18:00 H 2032

Synthesis and Stability of Indium (III) Oxide Polymorphs — •Aleksander Gurlo and Maged Bekheet — Fachgebiet Keramische Werkstoffe, Technische Universität Berlin, Fakultät III Prozesswissenschaften, Institut für Werkstoffwissenschaften und -technologien, Sekr. BA3, Hardenbergstraße 40, 10623 Berlin, Germany

In our presentation the synthesis, stability and properties of binary indium oxides will be addressed. Our recent works deal with the synthesis and characterization of the known and new polymorphs in indium-oxygen system. In this way (i) a new orthorhombic In2O3 polymorph has been synthesized under high-pressure high-temperature conditions and recovered to ambient pressure and temperature, (ii) the metastability of corundum-type In2O3 have been proved both theoretically and experimentally, (iii) new sol-gel methodologies to synthesize high pressure In2O3 polymorphs under ambient pressure conditions have been developed, (iv) the stabilisation of pseudo-cubic {012} morphology in corundum-type In2O3 over several length scales have been verified, (v) the mobility and carrier concentration of well-defined corundum- and bixbyite-type In2O3 nanocrystals have been measured at different temperatures and in different gas atmospheres, (vi) a synthetic methodology for hierarchically organized hollow spheres has been developed, (vii) the crystallization of bixbyite-type In2O3 has been proven using in-situ time-resolved synchrotron radiation, and (viii) the stabilization of high-pressure corundum-type In2O3 polymorph in nanocrystals have been explained.

HL 83.11 Thu 18:30 H 2032

Photocatalysis of Titania Thin Films Prepared by Sputtering versus Evaporation — Bodo Henkel[1], Thomas Neubert[2], Sebastian Zabel[1], •Thomas Strunskus[1], Michael Vergöhl[2], and Franz Faupel[1] — [1]Lehrstuhl für Materialverbunde, Institut für Materialwissenschaft, Christian Albrechts Universität zu Kiel — [2]Fraunhofer Institut für Oberflächen- und Schichttechnologie, Braunschweig

To achieve a deeper understanding about reasons for differing photocatalytic efficiencies of titania thin films made by different physical vapor deposition techniques, different grain and phase growth pathways of these titania thin films have been studied. Results are shown for two well established and widely used PVD methods, namely electron beam evaporation and reactive pulsed DC magnetron sputtering. In addition the effect of inducing oxygen vacancy defects by tempering in reducing atmospheres on their photocatalytic efficiency have been tested, as well as aging of these thin films. These titania thin films where characterized with respect to crystallinity, texture and phases (XRD and Raman), roughness and surface area (AFM), light transmission and band gap energy (UV-Vis), refractive index (Ellipsometry), film thickness (Profilometer, Ellipsometry, SEM cross section), grain growth and structure (AFM, SEM of surface and cross section) and photocatalytic efficiency (methylene blue degradation). Results show different nucleation and growth mechanisms for evaporated compared to sputtered titania thin films, which have severe influence on photocatalytic efficiency.

HL 83.12 Thu 18:45 H 2032

Interdependence of electroformation and hydrogen incorporation in titanium dioxide — Mara Strungaru[1], Mihai Cerchez[2], •Svenja Herbertz[2], Thomas Heinzel[2], Mhamed El Achhab[3], and Klaus Schierbaum[3] — [1]Faculty of Physics, Alexandru Ioan Cuza University, 700506, Iasi, Romania — [2]Solid State Physics Laboratory, Heinrich-Heine-Universität Düsseldorf — [3]Materials Science Laboratory, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf

Nanoporous titanium dioxide films are exposed to molecular hydrogen gas during electroformation. In addition to the usual reversible increase of the conductance of the films as hydrogen is offered, an irreversible decrease of the conductance is observed. The behavior is interpreted in terms of a phenomenological model where current carrying, oxygen-deficient filaments form inside the TiO_2 matrix in which hydrogen incorporation decreases the carrier density.

[1] M. Cerchez, H. Langer, M. E. Achhab, T. Heinzel, D. Ostermann, H. Lüder, and D. Ostermann, Appl. Phys. Lett. 103, 033522 (2013). [2] D. B. Strukov, G. S. Snider, D. R. Stewart, and R. S. Williams, Nature 453, 80 (2008). [3] T. Bjørheim, S. Stølen, and T. Norby, Phys. Chem. Chem. Phys. 12, 6817 (2010).