O 13: Focus Session: Crystalline n-type semiconducting oxides - SnO_2, Ga_2O_3, and In_2O_3 for novel devices (jointly with HL)

Traditionally, wide band gap semiconducting oxides have been synthesized as thin polycrystalline films for mainly passive components such as transparent conducting electrodes or gas sensors. More recently, however, it has been recognized that — highly pure and single-crystalline — these oxides can become semiconductor materials for active devices. Development of high quality oxides allows to study their intrinsic physics and enables potential applications in transparent (opto)electronics, power electronics, photonics, and chemical and biological sensors. This session sets a focus on crystalline SnO_2, Ga_2O_3, and In_2O_3 as n-type semiconducting oxides and gives a state-of-the-art survey of their physics including the prospects of applications. (Organizers: Oliver Bierwagen, PDI Berlin, and Saskia Fischer, HU Berlin)

Time: Monday 15:00–19:20 Location: H2

Topical Talk O 13.1 Mon 15:00 H2

Optical absorption and radiation damage in transparent conducting oxides — •Andre Schleife[1], Friedhelm Bechstedt[2], Alfredo Correa[1], and Yosuke Kanai[3] — [1]Lawrence Livermore National Laboratory — [2]Friedrich-Schiller-University Jena — [3]University of North Carolina at Chapel Hill

Transparent conducting oxides are promising semiconductors with important technological applications in various areas of optoelectronics and photovoltaics. An accurate description of *electronic excitations and their dynamics* is crucial for predictive materials design: Outer-space applications, for instance, not only require fundamental understanding of optical absorption but also of radiation damage.

This talk outlines how parameter-free computational electronic-structure techniques based on many-body perturbation theory accomplish the scientific challenge of describing the quantum-mechanical many-body nature of the electron-electron interaction. Insight will be provided into quasiparticle and excitonic effects affecting optical properties of magnesium-, cadmium, and tin-oxide compounds. The impact of free electrons on the optical band gap will be discussed as an important real-structure effect, e.g. in n-doped cadmium oxide.

In addition, this talk will outline high-performance first-principles computational schemes for accurately characterizing non-adiabatic dynamics of electrons and nuclei: Understanding the *electronic stopping* and defects, e.g. when fast hydrogen atoms penetrate magnesium oxide, is essential for developing materials with high radiation resistance. Partly prepared by LLNL under Contract DE-AC52-07NA27344.

O 13.2 Mon 15:30 H2

Anisotropic dielectric function and carrier density of rutile SnO_2 — •Christian Lidig[1], Karsten Lange[1], Martin Feneberg[1], Maciej Neumann[2], Norbert Esser[2], Mark E. White[3], Min-Ying Tsai[3], Oliver Bierwagen[3,4], James S. Speck[3], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung für Materialphysik — [2]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V. , Berlin — [3]University of California, Santa Barbara, USA — [4]Paul-Drude-Institut, Berlin

The anisotropic dielectric function of rutile SnO_2 is presented from 0.04 eV up to 20 eV. The results were obtained on a sample grown on TiO_2 having the optical axis in plane. After modelling the layer stack and taking surface roughness into account, the full dielectric function is extracted wich is compared with theoretical calculations. It turns out that electron-hole interaction influences the dielectric function up to 20 eV resulting in a pronounced redshift and redistribution of oscillator strength of features related to van Hove singularities.
Additionally, infrared spectroscopic ellipsometry was performed on a series of SnO_2:Sb layers grown on r-plane sapphire. The plasmon-longitudinal optical phonon- coupling modes yield results for the free carrier concentrations which are discussed in detail.

Topical Talk O 13.3 Mon 15:45 H2

Growth from the melt of high-quality In2O3 and Ga2O3 single crystals — •Roberto Fornari, Zbigniew Galazka, Reinhard Uecker, and Klaus Irmscher — Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin

Because of their interesting properties semiconducting oxides, in particular Ga2O3 and In2O3, have recently received much attention. However, as they were deposited as films on hetero-substrates their quality was quite poor. The growth of high-quality bulk Ga2O3 and In2O3 and manufacture of the corresponding substrates can allow the deposition of high-quality epilayers with lower residual carrier density and fewer extended defects. For this reason IKZ has undertaken an effort to grow large single crystals of these oxide compounds from the melt. Transparent semiconducting Ga2O3 single crystals with diameter of about 20 mm and 50-60 mm long were grown by the Czochralski method along the b-axis, using an Iridium crucible and a dynamic protective atmosphere to minimize the dissociation of Ga2O3 melt and ingot. In the case of In2O3 the Czochralski technique is not applicable and it was necessary to develop a novel melt growth method. This new method indeed supplied crystals from which oriented substrates could be prepared. In this presentation the melt growth of Ga2O3 and In2O3 single crystals will be reviewed. An important feature of both materials is given by their strong sensitivity to thermal processing: the free carrier concentration and the absorption spectra drastically vary as a function of annealing temperature, duration and ambient. The possible causes will be discussed.

Coffee break

O 13.4 Mon 16:30 H2

Surface structure of metal oxides via Fast Atom Diffraction — •Marco Busch[1], Eric Meyer[1], Jan Seifert[1], Helmut Winter[1], Klaus Irmscher[2], Zbigniew Galazka[2], and Roberto Fornari[2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, D-12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, D-12489 Berlin, Germany

Fast light atoms (H and ^{4}He) and molecules (H_2) with energies from 200 eV up to several keV are grazingly scattered from clean and flat surfaces. For scattering along low-indexed axial channels, we observe defined diffraction patterns in the angular distributions of scattered projectiles, which can be ascribed to Fast Atom Diffraction (FAD) with de Broglie wavelengths as low as about 10^{-3} Å. As example, we have investigated the quantum scattering from the cleaved (100) surface of a Ga_2O_3 single crystal, grown by the Czochralski method following by in situ annealing. The splittings of Bragg peaks and their intensity modulations were so far exploited to deduce information on the arrangement of atoms in the topmost surface layer. Furthermore, diffraction effects were present in the regime of surface channeling, where quantum scattering is considered for the motion parallel to the surface. For the $Al_2O_3(11\bar{2}0)$ surface we found, that beside the *normal coherence* also the *longitudinal coherence* is preserved, so that *Laue circles* are observed. Then, quantum scattering from surfaces gives rise to interesting features and enhances the resolution of FAD by one order of magnitude. As example, we have resolved the (12x4) superstructure on the $Al_2O_3(11\bar{2}0)$ surface obtained after annealing to about 2000 K.

Topical Talk O 13.5 Mon 16:45 H2

Development of gallium oxide power devices — •Masataka Higashiwaki[1,2], Kohei Sasaki[1,3], Akito Kuramata[3], Takekazu Masui[4], and Shigenobu Yamakoshi[3] — [1]National Institute of Information and Communications Technology, Koganei, Tokyo, Japan — [2]JST PREST, Chiyoda, Tokyo, Japan — [3]Tamura Corporation, Sayama, Saitama, Japan — [4]Koha Co., Ltd., Nerima, Tokyo, Japan

Gallium oxide (Ga_2O_3) has excellent material properties for power device applications represented by the extremely large breakdown field of 8 MV/cm due to a large band gap of 4.8–4.9 eV. Another important feature in industry is that large single-crystal β-Ga_2O_3 bulks can be fabricated with melt-growth methods. We recently succeeded in fabricating Ga_2O_3 metal-semiconductor field-effect transistors (MES-

FETs) and Schottky barrier diodes (SBDs) on single-crystal β-Ga_2O_3 substrates by using newly developed technologies for making single-crystal substrates, growing conductivity-controlled epitaxial films, and fabricating devices. The MESFETs exhibited excellent device characteristics including an off-state breakdown voltage (V_{br}) over 250 V, an extremely low leakage current (several μA/mm), and a high on/off drain current ratio of around 10,000. The SBDs also showed good characteristics such as an ideal factor very close to 1.0 and a high reverse V_{br}. These results indicate that Ga_2O_3 have comparable or even more potential than Si and typical widegap semiconductors SiC and GaN for power device applications.

O 13.6 Mon 17:15 H2

Structural, optical and electrical properties of Si-doped β-β-Ga_2O_3 thin films — •Stefan Müller, Holger von Wenckstern, Florian Schmidt, Daniel Splith, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

The wide bandgap oxide semiconductor β-Ga_2O_3 (E_g = 4.9 eV at room temperature) is a promising material for realization of transparent optoelectronics like FETs [1] or solar-blind photodetectors.
In this contribution we present structural, optical and electrical properties of 1% SiO_2-doped β-Ga_2O_3 thin films grown by pulsed-laser deposition (PLD) on *c*-plane sapphire substrates. The oxygen partial pressure was set between 3×10^{-4} and 0.024 mbar and the substrate temperature between 570°C and 730°C. The thin films are $(\bar{2}01)$-oriented if grown at low oxygen partial pressures and high temperatures. At a growth temperature of 730°C and for oxygen partial pressures above 10^{-3} mbar additional orientations are visible in the XRD pattern. The transmissivity between 1100 nm and 280 nm is in the range of 80% for most investigated samples. However, the optical bandgap increases from 4.7 eV (0.04 mbar) to 4.9 eV (3×10^{-4} mbar) with decreasing oxygen partial pressure. The maximal conductivity and electron mobility of our thin films is in the range of 20 S/m and 0.15 cm^2/Vs, respectively.
[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).

O 13.7 Mon 17:30 H2

Schottky contacts on β-Ga_2O_3 thin films grown by pulsed laser deposition — •Daniel Splith, Stefan Müller, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

A promising oxide semiconductor for high power electronics and transparent optoelectronic devices is β-gallium oxide (Ga_2O_3) with a band gap of about 4.9 eV. We have investigated the preparation and the properties of Schottky contacts (SCs) on Ga_2O_3 thin films. The thin films were grown from a Ga_2O_3 target with 1% SiO_2 on c-sapphire substrates using pulsed-laser deposition at an oxygen pressure of 10^{-3} mbar. The ohmic contacts were fabricated by thermal evaporation of Ti and Al as reported in [1]. Subsequently, we prepared SCs by normal and reactive DC sputtering of metals like Nb, W or Cu. The $I-V$ characteristics of such SCs showed rectification ratios up to 8 orders of magnitude for some of the Nb contacts. The dominant current transport mechanism is thermionic emission. From fits we determined ideality factors n down to 1.15 for the best W contacts and barrier heights Φ_B up to 1.2 eV for the best Cu contacts. Temperature dependent $I-V$ measurements yielded a linear dependence of Φ_B and $\frac{1}{n}-1$ on the inverse temperature in accordance to the theory of thermionic emission in the presence of a laterally inhomogeneous barrier. E. g. the mean barrier height $\overline{\Phi}_B$ for the Cu contacts is determined to be 1.6 eV with a standard deviation σ_Φ of 0.17 eV.
[1] E. G. Villora *et al.*, Appl. Phys. Lett. 92, 202118 (2008)

Coffee break

O 13.8 Mon 18:00 H2

Printed, high performance inorganic oxide transistors from halide precursors — •Suresh Kumar Garlapati[1,2], Nilesha Mishra[1], Ramona Hahn[1], Simone Dehm[1], Robert Kruk[1], Subho Dasgupta[1], and Horst Hahn[1,2,3] — [1]Institute for nanotechnology, Karlsruhe institute of technology(KIT) ,Eggenstein, Germany — [2]KIT-TUD Joint research laboratory nanomaterials, TU Darmstadt, Darmstadt, Germany — [3]Center for functional nanostructures, KIT, Germany

Ink-jet printed field-effect transistors (FETs) are recently of great interest for large area electronics; especially when they exhibit high field-effect mobility. The importance of such devices increases even further when they are operated with very low voltages and compatible to portable electronic applications. However, examples of low voltage driven, high mobility FETs that are scalable for high volume production is scarce in the literature. Here, we report ink-jet printed, halide precursor based extremely high mobility oxide (In2O3) FETs that are gated with composite solid polymer electrolytes to limit the operation voltage to 1 V. The printed precursors have been annealed at different temperatures (573-773 K) and as a result devices have shown little dissimilar performance depending on the degree of crystallization and size of crystallites. Nevertheless, the performance for the lowest temperature annealed devices (573 K) has also been quite outstanding; device mobility close to 50 cm^2V^-1s^-1 and On/Off ratio in excess of 10^5 is noted. The achieved field-effect mobility ensures high semiconductor quality and excellent semiconductor/dielectric interface.

Topical Talk O 13.9 Mon 18:15 H2

Surface electron accumulation layers in oxide semiconductors — •Tim Veal — University of Liverpool, Liverpool, UK

In contrast to the electron depletion at the surface of almost all n-type semiconductors, electron accumulation has long been known to occur at ZnO surfaces. It has recently been found to be characteric of several other oxide semiconductors, including CdO [1,2], In_2O_3 [3] and SnO_2. They all have a significant size and electronegativity mismatch between their cation and anion. As a result, they have a particularly low Γ-point conduction band minimum which is ultimately responsible for the propensity for electron accumulation. As well as the existence of an electron-rich layer, it has been found, using angle-resolved photoemission spectroscopy (ARPES), to be quantized into 2D subbands [1]. Moreover, the conventional one-electron picture of surface space-charge in semiconductors is shown to be inconsistent with the electronic structure observed directly from ARPES, indicating that many-body interactions play a large role in the surface electronic properties of these oxides. Such interactions lead to a depth-dependent shrinkage of the semiconductor band gap, resulting in a surface band gap which differs from the bulk value [1]. The most recent studies have focussed on the influence of depositing alkali metals onto these surfaces. Many collaborators are acknowledged for samples and ARPES expertise.
[1] P. D. C. King, T. D. Veal *et al.*, PRL **104**, 256803 (2010); [2] P. D. C. King, T. D. Veal *et al.*, PRB **79**, 035203 (2009); [3] P. D. C. King, T. D. Veal *et al.*, PRL **101**, 116808 (2008)

O 13.10 Mon 18:45 H2

Surface and bulk derived in-gap states of In_2O_3 single crystals — •Dorothee Braun[1], Valentina Scherer[1], Christoph Janowitz[1], Zbigniew Galazka[2], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

The influence of intrinsic point defects on the electronic structure of n-type In_2O_3 single crystals grown by two methods, namely chemical vapor transport (CVT) and melt growth, was examined by two different spectroscopic methods. First, with scanning tunneling spectroscopy (STS), a very surface sensitive technique for measuring the local density of states (LDOS). So far not resolved states within the fundamental band gap have been observed. The gap states have been studied for different crystals and after several temper treatments in oxygen. Second, low-energy angular-resolved photoemission spectroscopy (low-e ARPES) at $h\nu = 9$ eV photon energy has been used to investigate the gap states in the bulk. In contrast to conventional ARPES at typical VUV we were now able to resolve individual emissions of the gap states as well as their momentum dependence. The spectroscopic results will be compared to state of the art DFT-calculations revealing the origin of the gap states in In_2O_3 to be due to oxygen vacancies as well as indium and oxygen interstitials.

O 13.11 Mon 19:00 H2

Electron transport in molecular-beam-epitaxy-grown SnO_2 and In_2O_3 films: Doping, defects, and the surface — •Oliver Bierwagen[1,2], Natalie Preissler[1], Takahiro Nagata[2,3], Mark E. White[2], Min-Ying Tsai[2], and James S. Speck[2] — [1]Paul-Drude-Institut, Berlin, Germany — [2]University of California, Santa Barbara, USA — [3]National Institute for Material Science, Tsukuba

Electron transport and its control are key issues for the application of semiconducting oxides in (opto)electronic devices. To this end, the

electron transport in unintentionally- and intentionally doped, high quality, molecular-beam-epitaxy-grown tin oxide (SnO_2) and indium oxide (In_2O_3) films is reviewed.[1] Comparably high mobilities indicate high purity and quality.[2] The resistivity was successfully varied over more than seven orders of magnitude from a transparent conducting oxide-like conductivity by donor doping up to the semi-insulating range (but no p-type conductivity) by acceptor doping.[3,4] Oxygen-related defects play a critical role in In_2O_3.[2, 4] A surface electron accumulation layer is present in both oxides.[5,6] While it strongly influences contact properties,[6,7] its conductance is negligible.[3,6]

[1] O. Bierwagen et al.*Chapter 15 - MBE of transparent semiconducting oxides* in *Molecular Beam Epitaxy*, Elsevier Oxford (2012).
[2] O. Bierwagen and J.S. Speck, Appl. Phys. Lett. 97, 072103 (2010).
[3] O. Bierwagen et al., J. Mater. Res. 27, 2232 (2012).
[4] O. Bierwagen and Speck, Appl. Phys. Lett. 101, 102107 (2012).
[5] T. Nagata et al., Appl. Phys. Lett. 98, 232107 (2011).
[6] O. Bierwagen et al., Appl. Phys. Lett. 98, 172101 (2011).
[7] O. Bierwagen et al., Appl. Phys. Express 2, 106502 (2009); T. Nagata et al. J. Appl. Phys. 107, 033707 (2010).

Concluding remarks