HL 69: Focussed Session: Oxide Semiconductors for Device and Energy Applications 1

Semiconducting metal oxides possess a very high potential for electronic devices and energy applications. For example, the n-type semiconductor Ga_2O_3 is currently intensively investigated due to its favorable semiconducor properties for power electronics, whereas the p-type semiconductor NiO can serve as important charge extraction barrier, to increase the efficiency of organic photovoltaics. The scope of this focus session encompasses well defined oxide structures of highest material quality and the understanding of their device-related physical properties as essential prerequisites for the application-relevant technological control of semiconducting metal oxides.

Organizers: Andreas Klein (TU Darmstadt), Oliver Bierwagen (PDI Berlin), Holger von Wenckstern (U Leipzig), and Martin Feneberg (OvGU Magdeburg)

Time: Thursday 9:30–13:15 Location: H11

Topical Talk HL 69.1 Thu 9:30 H11

Oxide semiconductors: materials design and applications — •Hideo Hosono — Tokyo Institute of Technology, Yokohama, Japan,

Oxide semiconductors have a long history comparable to IV group element semiconductors. Although industrial application remains still a few, industrial application of thin film transistors with oxide semiconductor (IGZO) channel has started to drive high resolution, large sized OLED-TVs as well as energy-saving LCDs recently, and Ga2O3 with a band gap of ~5eV is attracting as a semiconductor for power electronic applications.

The chemical bonding of oxides is rather different from that of typical semiconductors, which in turn gives unique band structure and crystal structure. In this talk, I review the progress of oxide semiconductors in last 2 decades focusing on materials design and applications utilizing the unique nature of oxides.

Topical Talk HL 69.2 Thu 10:15 H11

Mixing In and Ga sesquioxides - and their polar phases — •Vincenzo Fiorentini — Dept of Physics, Cagliari University, Italy — CNR-IOM, UOS Cagliari, Italy

This talks will report on recent first-principles theoretical work on the In and Ga sesquioxides and their ternary alloy, an up-and-coming materials system for near to deep-UV large-breakdown and transparent-conducting materials. Firstly, a qualitative phase diagram is proposed over all the full composition range. Three structures –monoclinicβ, layered-hexagonal, and cubic bixbyite– are competing for the ground state, and several regions of miscibility and phase separation interlace as function of composition, more or less independently of temperature. Electronic properties, including absorption anisotropy at low x, and a selection of interface band offsets will also be presented. Secondly, the metastable polar phase ε-Ga_2O_3 is shown to be pyroelectric (i.e. locked in a non-switchable polarized structure) with a large ferroelectric-like polarization 0.23 C/m^2 and a diagonal piezoelectric coefficient (0.77 C/m^2) in line with those of III-V nitrides and II-VI oxides. In view of recent growth successes in that direction, the interface of ε-Ga_2O_3 to GaN is studied, both in terms of geometry, offsets, and polarization difference, suggesting interesting potential for power applications.
Work in collaboration with M. B. Maccioni, F. Ricci, R. Fornari.

Topical Talk HL 69.3 Thu 10:45 H11

Exploring and tailoring conductance phenomena in oxide films: An STM study — •Niklas Nilius — Carl von Ossietzky Universität Oldenburg

Electronic properties of classical semiconductors, e.g. Si, are adjustable with high accuracy and form the basis of todays information technology. Also oxides exhibit fascinating electronic features, e.g. a large spread in gap sizes, a correlated electronic behavior, metal-insulator transitions, anomalous temperature and voltage dependencies and superconductivity. Despite this potential, no satisfactory mechanistic understanding of oxide properties has been achieved so far and preparation of phase-clean materials remains challenging.

My talk demonstrates how thin-film oxides of high structural quality can be prepared and explored at atomic length-scales by STM. The approach yields direct correlation between structural parameters and electronic properties of the materials. Moreover, their conductance behavior becomes tunable, e.g. by stoichiometry and defect engineering, doping and interface control. I will present examples for low-gap oxides, e.g. Cu_2O and V_2O_3, and discuss how their electronic response is affected by intrinsic defects and dopants. For wide-gap materials, such as MgO and CeO_2, the interplay between conductance and low-dimensional edge and surface states as well as uncompensated polarity is addressed. Finally, the transition from binary to ternary oxides is introduced as a route to tune electronic properties. My talk aims at providing mechanistic insights into the structure-conductivity relationship rather than presenting materials of direct technological relevance.

15 min. break.

Topical Talk HL 69.4 Thu 11:30 H11

Miscibility and phase separation in $(In_xGa_{1-x})_2O_3$ — •Martin Albrecht[1], Robert Schewski[1], Toni Markurt[1], Tobias Schulz[1], Michele Baldini[1], Günter Wagner[1], Holger von Wenckstern[2], Marius Grundmann[2], Hartwin Peelaers[3], Joel Varley[3], and Chris Van de Walle[3] — [1]Institute for Crystal Growth, Berlin, Germany — [2]Universität Leipzig — [3]Materials Department, University of California, Santa Barbara, California, USA

Group III sesquioxides are distinguished from other wide band gap semiconductors by the fact, that they can be efficiently n-doped despite a wide band gap that ranges from 2.7 eV for In_2O_3 over 4.8 eV for Ga_2O_3 to 8.9 eV for Al_2O_3. Full exploitation of their properties for electronic applications requires band gap engineering formation of solid solutions. The formation of solid solutions in group III sesquioxides is challenging, since, at thermodynamic equilibrium, the binaries exhibit different thermodynamically stable structures (cubic, rhombohedral, and monoclinic) besides a significant lattice mismatch. The oxygen coordination of the metal atoms in the binary alloys is either octahedral, or mixed tetrahedral and octahedral. In this presentation we report on transmission electron microscopy studies on miscibility and phase separation in the system $(In_xGa_{1-x})_2O_3$ grown by PLD. We identify essentially three different phases as dependent on composition, i.e. the monoclinic β-phase in the compositional range up to $x = 0.5$, an ordered hexagonal phase in the range between $x = 0.5$ and 0.75 and the cubic bixbyite phase at higher In contents. In atoms occupy octahedrally coordinated cation sites in the monoclinic phase.

HL 69.5 Thu 12:00 H11

Infrared response of cubic In_2O_3 — •Martin Feneberg[1], Christian Lidig[1], Jakob Nixdorf[1], Oliver Bierwagen[2,3], James S. Speck[3], Zbigniew Galazka[4], and Rüdiger Goldhahn[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke Universität Magdeburg — [2]Paul Drude Institut für Festkörperelektronik, Berlin — [3]Materials Department, University of California, Santa Barbara, USA — [4]Leibniz-Institut für Kristallzüchtung, Berlin

The infrared optical response of cubic bixbyite In_2O_3 samples is investigated in detail. Samples with different concentrations of free electrons from 1.5×10^{17} up to 1.6×10^{21} cm^{-3} are measured by spectroscopic ellispometry yielding dielectric functions. Besides transerse optical phonon modes a Drude contribution accounting for the free electron gas is observed and analyzed.

The broadening factor in the Drude contribution can be understood as characteristic relaxation time constant. Its frequency dependency is visible in point-by-point fitted dielectric functions, i.e. without assumptions about the line shape. The broadening factor is found to be a constant within errors of measurement.

By comparison with Hall-effect data, the effective electron mass is found to be a function of energy increasing from $m^* = 0.18m_0$ at the Γ-point of the Brillouin zone. This is direct proof of the non-parabolic nature of the conduction band.

HL 69.6 Thu 12:15 H11

Electrical conductivity and gas-response of the In_2O_3 surface electron accumulation layer — •Julius Rombach[1], Oliver Bierwagen[1], Alexandra Papadogianni[1], Markus Mischo[2], Volker Cimalla[2], Oliver Ambacher[3], Theresa Berthold[4], Marcel Himmerlich[4], and Stefan Krischok[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin — [2]Fraunhofer Institut für Angewandte Festkörperphysik, Freiburg — [3]Institut für Mikrosystemtechnik, Freiburg — [4]Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany

Indium oxide is a well-known material for conductometric gas sensors, showing a decrease in conductance when exposed to oxidizing gases. In contrast to typically used polycrystalline films, we study MBE-grown single-crystalline In_2O_3 thin films as a model system with reduced complexity. Electrical conductivity of these films essentially consists of two parallel contributions: the bulk of the film and the surface electron accumulation layer (SEAL) of unknown conductance. Both these contributions are varied to understand their effect on the sensor response. Conductivity changes induced by UV illumination in air, forcing desorption of oxygen adatoms on the surface, and gas-response measurements in ozone atmosphere give a measure of the sensor response and show that the sensor effect is only due to the SEAL conductivity. Therefore, a strong sensitivity increase is achieved by reducing the bulk (or intra-grain) conductivity. Hall and Seebeck measurements will give further details helping to estimate the SEAL electron concentration and mobility.

HL 69.7 Thu 12:30 H11

Surface structure of β-Ga_2O_3(100) via classical and quantum mechanical rainbow scattering — •Marco Busch[1], Eric Meyer[1], Helmut Winter[1], Zbigniew Galazka[2], Klaus Irmscher[2], and Konrad Gärtner[3] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, 12489 Berlin, Germany — [3]Institut für Fest- körperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Fast light atoms and molecules with energies from 200 eV up to several tens of keV are grazingly scattered from a clean and well-ordered β-Ga_2O_3(100) surface. The angular distributions of projectiles scattered in the regime of axial surface channeling show intensity maxima, which can be described with the concept of the classical rainbow scattering and offer the determination of the interaction surface potential. However, for decreasing projectile energy one can observe Bragg peaks in the angular distributions, which can be interpreted within the framework of quantum mechanics only. Here, we present investigations of the quantum scattering from the ex-situ cleaved and in-situ annealed (100) surface of β-Ga_2O_3 single crystals, grown by the Czochralski method. The splittings of Bragg peaks and their intensity modulations were so far exploited to deduce information on the arrangement of the atoms and thereby the termination and relaxation of the topmost surface layer [1]. Based on these investigations, the adsorption of atoms and molecules on the β-Ga_2O_3(100) surface can be studied in detail. [1] M. Busch et al., Appl. Phys. Lett. **105**, 051603 (2014).

HL 69.8 Thu 12:45 H11

Vibrational spectra, Raman and IR properties of Copper-Oxide Phases from first principles — •Marcel Giar, Markus Heinemann, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Vibrational properties of the three copper oxide phases Cu_2O, Cu_4O_3, and CuO are derived from DFT calculations. Phonon dispersions including non-analytical contributions to the dynamical matrix in the limit $\mathbf{q} \to \mathbf{0}$ are presented as well as derived quantities such as acoustic phonon group velocities and thermodynamics. We further examine Raman and IR properties and their behavior under uniform external pressure. The frequency dependence of the Raman susceptibility and resulting changes in the Raman scattering intensities are also assessed.

HL 69.9 Thu 13:00 H11

Optical properties of single crystalline $SrMoO_3$ thin films — •Aldin Radetinac, Jörg Zimmermann, Karoline Hoyer, Hongbin Zhang, Philipp Komissinskiy, and Lambert Alff — Institute for Materials Science, TU Darmstadt, Germany

The optical properties of pulsed laser deposited highly crystalline $SrMoO_3$ thin films were investigated.[1] Due to their low resistivity below 30 $\mu\Omega$cm, thin films of $SrMoO_3$ are candidates for transparent conductor applications. The transparency of $SrMoO_3$ extends into the ultraviolet range to about 300 nm. In this range, $SrMoO_3$ has a higher transparency at similar sheet resistance as compared to alternative oxide or metallic materials. Density functional theory shows that electron-electron correlation effects are small in $SrMoO_3$ as compared to other low-resistivity transition metal oxides and predicts the optical properties in good agreement with experiment. This work was supported by the DFG project KO 4093/1-1.

[1] A. Radetinac, J. Zimmermann, K. Hoyer, H. Zhang, P. Komissinskiy and L. Alff submitted to J. Appl. Phys. (2015)