O 4: Focussed session: Transparent conductive oxides I (jointly with HL, DS)

Time: Monday 11:15–13:00 Location: WIL A317

Topical Talk O 4.1 Mon 11:15 WIL A317

Surface and Bulk Properties of Post-Transition Metal Oxide Semiconductors — Philip D.C. King, Sepehr Vasheghani Farahani, Tim D. Veal, and •Chris F. McConville — Department of Physics, University of Warwick, Coventry, CV4 7AL UK

Oxide semiconductors have become of great interest lately with enormous opportunities for new uses that will potentially improve existing materials and device applications. The fact that some of these materials, such indium tin oxide, in a relatively low quality form, have seen significant industrial use as transparent conductors has perhaps contributed to the belated recognition of the possibilities as semiconductors in their purer form. Here, the surface and bulk electronic properties of epitaxially grown high-quality oxide semiconductors (In_2O_3, CdO, and ZnO) will be discussed. Optical, electronic and structural properties of these semiconducting oxide films will be presented. The valence band density of states and the surface electronic properties of these oxide semiconductors have been studied using high-resolution photoemission spectroscopy and compared with theoretical band structure calculations. A common property of these oxide semiconductors is found to be the presence of a surface electron accumulation layer, in marked contrast to the electron depletion generally observed at the surfaces of conventional semiconductors. Additionally, hydrogen is found to be a donor and any native defects have a propensity to be donors in already n-type material. The origin of these phenomena will be discussed in terms of the band structure and intrinsic properties of these materials.

Topical Talk O 4.2 Mon 11:45 WIL A317

***Ab-initio* calculation of electronic and optical properties of transparent conductive oxides** — •André Schleife[1,3], Claudia Rödl[1], Frank Fuchs[1], Jürgen Furthmüller[1], Benjamin Höffling[1], Karsten Hannewald[1], Patrick Rinke[2], Joel Varley[3], Anderson Janotti[3], Chris G. Van de Walle[3], and Friedhelm Bechstedt[1] — [1]IFTO and ETSF, FSU Jena, Germany — [2]FHI and ETSF, Berlin, Germany — [3]Materials Department, UC Santa Barbara, USA

Parameter-free calculations are a modern and sophisticated complement to advanced experimental techniques when exploring the properties of materials. Due to the rapidly increasing computing power they promise a deep understanding of the underlying physics also for more complex transparent conductive oxides.

We take the excitation aspect of photoemission processes into account by calculating the quasiparticle electronic structure using the modern HSE03+G_0W_0 framework. Solving a Bethe-Salpeter equation for the optical polarization function allows us to account for excitonic and local-field effects that govern the optical absorption.

After an introduction into these recent theoretical-spectroscopy techniques we apply them to ZnO, SnO_2, In_2O_3, and Ga_2O_3. We present results for the electronic band structure (including spin-orbit coupling), the band alignment, dielectric functions, exciton binding energies, and optical oscillator strengths. The influence of a degenerate electron gas, which occurs in these typically n-type materials, is investigated. Our findings are discussed with respect to available experimental results.

Topical Talk O 4.3 Mon 12:15 WIL A317

Bulk semiconducting oxides: crystal growth and physical properties — •Roberto Fornari — Leibniz Institute for Crystal Growth, IKZ, Max-Born-Str. 2, 12489 Berlin

Semiconducting oxides have attracted considerable interest in the last few years. In addition to the widely studied ZnO, much attention has recently been devoted to Ga2O3, In2O3 and SnO2. The epitaxial growth has already been achieved on different hetero-substrates; however due to the relatively poor crystallographic quality of the obtained layers it was not possible to get devices or even reliably measure their physical properties so far. It is thus urgent to provide homo-substrates which may allow the deposition of high-quality epilayers with low residual carrier density and fewer extended defects. IKZ has recently undertaken an effort to grow large single crystals of these oxide compounds. In this presentation the growth of transparent semiconducting Ga2O3 single crystals will be reviewed. Single crystals with diameter of 18 mm diameter and 50-60 mm length were grown along the b-axis from an Iridium crucible under a dynamic protective atmosphere. The transmission in IR-region was directly correlated with the free carrier concentration and was found to depend on the growth atmosphere and/or post growth annealing. Typical electrical properties at room temperature are: resistivity = 0.12 Ohmcm, electron concentration = 2-5E17 cm-3 and mobility = 110 cm2/Vs; these results seem to derive from a donor level with activation energy of about 32 meV. Results of thermodynamic calculations, dislocation density studies, ICP-OMS, DTA, EPR and High Resolution TEM are also presented.

O 4.4 Mon 12:45 WIL A317

The electronic properties of β -Ga_2O_3 — •Mansour Mohamed[1], Christoph Janowitz[1], Isaak Unger[1], Zbigniew Galazka[2], Justin R. Weber[3], 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 — [3]Materials Department, University of California, Santa Barbara, California 93106-5050, USA

Ga_2O_3 belongs to the group of transparent conducting oxides (TCOs) with a wide band gap. It exhibits the largest band gap with E_g = 4.9 eV [1] and thus a unique transparency from the visible into the UV region. The n-type high-quality β -Ga_2O_3 single crystals were grown by the Czochralski method [2]. The crystals were characterized by different techniques (LEED, STM). The experimental valence band structure of β-Ga_2O_3 was determined by high-resolution angle-resolved photoelectron spectroscopy (ARPES) utilizing synchrotron radiation. The calculated band structure was determined using advanced density functional theory (DFT) calculations employing hybrid functionals and projector augmented wave (PAW) potentials. From theory, we obtained a direct band gap of 4.87 eV and a slightly smaller indirect band gap of 4.83 eV, with the valence-band maximum (VBM) located slightly away from the M symmetry point. The experimental band structure of β-Ga_2O_3 is compared and discussed with the theoretical calculations. The effect of changing the temperature from 300K to 20K on the experimental band structure β-Ga_2O_3 was studied.