DS 30: Focus Session: Emerging oxide semiconductors II (jointly with HL, DF, O)

Continuation of the morning session 'Emerging oxide semiconductors I'

Organizers: Oliver Bierwagen, Paul-Drude-Institut für Festkörperelektronik, Berlin, Norber Esser, Leibniz-Institut für Analytische Wissenschaften ISAS, Berlin, Rüdiger Goldhahn, Otto von-Guericke-Universität Magdeburg, and Marius Grundmann, Universität Leipzig.

Time: Wednesday 15:00–18:45 Location: POT 081

Topical Talk DS 30.1 Wed 15:00 POT 081

Electronic properties of the transparent semiconducting oxides Ga2O3 and In2O3 — •Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

The exploration of oxides from the perspective of semiconductor science and technology offers great opportunities for uncovering new physics as well as developing novel devices with unprecedented performance and functionality. In this talk the transparent semiconducting oxides (TSO) Ga2O3 and In2O3 will be presented. Regarding the electronic structure respectively band structure, crucial progress has been reached in the last years. Here Ga2O3 and, in particular, the (100) surface behaves like expected for a large-gap semiconductor. Against this, for In2O3 the occurrence of a charge accumulation layer is heavily debated. This possibly will restrict their potential for applications.

DS 30.2 Wed 15:30 POT 081

Dielectric function of In_2O_3 from the mid-infrared into the vacuum ultraviolet — •Rüdiger Goldhahn[1], Jakob Nixdorf[1], Christian Lidig[1], Klaus Irmscher[2], Zbigniew Gałazka[2], Oliver Bierwagen[3,4], James S. Speck[4], Christoph Cobet[5], and Martin Feneberg[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — [2]Leibniz-Institut für Kristallzüchtung, Berlin — [3]Paul Drude Institut für Festkörperelektronik — [4]University of California, Santa Barbara — [5]Johannes Kepler Universität, Linz

The optical properties of cubic bixbyite In_2O_3 are under intense discussion. There is not even a consensus about the direct or indirect nature of the fundamental band gap and the corresponding energies. Here, we present spectroscopic ellipsometry from the phonon region in the mid-infrared up to 10 eV using several different instruments including synchrotron radiation. The studies comprise bulk (111) crystals and epitaxial (001) thin films on (001) yttria-stabilized zirconia covering a wide range of electron concentrations (N_s). The dielectric function of In_2O_3 at high energies exhibits pronounced features related to critical points. By analyzing certain peculiarities of ellipsometric data, the fundamental band gap energy to be 2.77 ± 0.02 eV for low N_s. A continuous Burstein-Moss shift is found for increasing N_s. The analysis of the plasma frequency yields an electron effective mass of about $0.23m_0$.

DS 30.3 Wed 15:45 POT 081

Barrier height of Ag on In_2O_3 (111) single crystals — •maryam nazarzadehmoafi[1], stephan machulik[1], florian Neske[1], christoph janowitz[1], zbigniew galazka[2], and recardo manzke[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, Berlin, Germany

The barrier height of a metal-semiconductor contact was studied by means of angle-resolved photoemission spectroscopy, which was implemented through stepwise Ag deposition on the (111) surface of In_2O_3 single crystals. Work function of Ag and electron affinity of In_2O_3 were measured in situ, being 4.21 ± 0.05 eV and 4.24 ± 0.05 eV, respectively. A slight barrier height of 0.15 ± 0.07 eV was determined by following the band bending of valence band and core level spectra with Ag coverage. Good agreement was observed when comparing the results to a calculation of the height by applying the Schottky-Mott rule, yielding the negligible value of 0.03 ± 0.05 eV. Therefore, the character of the contact is ohmic like. Additionally, the results revealed the existence of diffuse band-gap states for In_2O_3(111) and a Fermi level shift by 0.09 ± 0.02 eV due to the photovoltage effect with Ag deposition.

DS 30.4 Wed 16:00 POT 081

Metal contacts on the beta-Ga2O3 single crystal (001) surface — •Stephan Machulik[1], Maryam Nazarzadehmoafi[1], Mansour Mohamed[2], Andreas Siebert[1], Christoph Janowitz[1], Zbigniew Galazka[3], and Recardo Manzke[1] — [1]Humboldt Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]Assiut University, Physics Department, Faculty of Science, Assiut 71516, Egypt — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, Berlin, Germany

Results of band structure measurements on beta-Ga2O3 single crystals were in good agreement with theoretical calculations [1], indicating a good theoretical understanding of this material. For application purposes in semiconductor technologies both Schottky and Ohmic metal-semiconductor contacts are required. ARPES and I/U measurements performed on n-doped Au-beta-Ga2O3(001) contacts confirmed Schottky-like behavior with a barrier height of 1.01 eV [2]. Motivated by the lower work function of silver we performed an ARPES study of Ag-beta-Ga2O3(001). The results point to a distinctly lower Schottky barrier, but the contact was not yet Ohmic. Additionally the work function depending on the layer thickness of Ag was studied.

[1] M. Mohamed, C. Janowitz, I. Unger, R. Manzke, Z. Galazka, R. Uecker, R. Fornari, J.R. Weber, J.B. Varley, C.G. van de Walle, Appl. Phys. Lett. 97, 211903 (2010)

[2] M. Mohamed, K. Irmscher, C. Janowitz, Z. Galazka, R. Manzke, R. Fornari, Appl. Phys. Lett. 101, 132106 (2012)

DS 30.5 Wed 16:15 POT 081

Sputtered SnO_2 degenerately doped with Ta or Sb - A comparative study for applications in transparent electronics — •Mirko Weidner and Andreas Klein — Technische Universität Darmstadt

In the emerging field of transparent electronics, indium oxide doped with tin (ITO) is still the predominately used electrode material, due to its high conductivity at low deposition temperatures. Due to the relative scarcity and high cost of Indium, alternatives are highly sought after. Tin oxide (SnO_2) is one of the few other materials that combine the properties of optical transparency and electrical conductivity. The material may serve as a transparent electrode in optoelectronic devices such as displays, touch screens, LEDs and thin film solar cells. In recent years, SnO_2 doped with Tantalum (TTO) has been shown to be a valid alternative to the established SnO_2 systems doped with Fluorine (FTO) or Antimony (ATO). However, little work has been published on the material, and thus far the question as to why Tantalum doping can yield better electrical conductivity than Antimony doping has not been raised or answered.
In this study, TTO and ATO thin films where sputter-deposited and characterized under similar conditions to maximize comparability between the two materials. Characterization of electrical conductivity and optical transmissivity was complimented by probing the materials' electronic structure by in-situ Photoelectron Spectroscopy (XPS/UPS) of the sample surfaces and by structural characterization by AFM and XRD.

DS 30.6 Wed 16:30 POT 081

Structural and electrical properties of Nb doped TiO_2 anatase films (2 - 17 at.%) sputtered with plasma emission control — •Sebastian Schipporeit[1], Sanat Kumar Mukherjee[1], Hans-Werner Becker[2], Andrew Paolo Cádiz Bedini[1], Christian Notthoff[1], Abdelkader Nebatti[1], Detlef Rogalla[1], Azadeh Soleimani-Estafani[1], and Dieter Mergel[1] — [1]Thin Film Technology Group, Faculty of Physics, University Duisburg-Essen — [2]University Bochum

Nb doped TiO_2 films were deposited using radio frequency magnetron sputtering with a metallic Ti target and introducing O_2 and Ar gas into the chamber. Nb wires were put onto the sputter track of the Ti target and the oxidation state of the target was controlled using a Ti line of the plasma emission. The films were analysed with XRD, RBS, SEM, EDX and XPS. After annealing at 400 °C, all films are polycrystalline and inhibit anatase structure. The Nb/(Nb+Ti) content varies from 2 to 17 at.%. The lattice parameter a and the unit cell volume

increase in a similar manner compared to TiO_2:Nb single crystals.

The films with the lowest resistivity of $7{\cdot}10^{-4}$ Ωcm (Nb content: 10 at.%) were coated with an oxidation state of the target in the transition region between metallic and oxidic modes. The Nb is incorporated as Nb^{5+} into the anatase lattice. In films with higher resistivity, the donor effect of Nb might be compensated by Ti vacancies (acceptors). The oxygen content is higher than in stoichiometric TiO_2. Ogyxen interstitials might increase the mass density in the films.

Coffee break (15 min.)

Topical Talk DS 30.7 Wed 17:00 POT 081

Surface properties of In_2O_3 and other semiconducting metal oxides — •Ulrike Diebold — Institute of Applied Physics, TU Vienna, Austria

The atomic-scale surface properties of semiconducting oxides influence, and often even dominate, their performance in a variety of applications. Often, local effects such as defects can severely affect the local electronic structure and surface chemistry. Our group uses STM in combination with DFT and area-averaging spectroscopies to investigate such phenomena at the atomic scale. Recent results on single crystalline In_2O_3 and other metal oxides will be discussed.

DS 30.8 Wed 17:30 POT 081

STM and STS at the InO(111) cleavage surface — Robert Zielinski, Andrea Lenz, Josephine Schuppang, Mario Dähne, and •Holger Eisele — Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany

The freshly cleaved In2O3(111) surface is investigated by UHV cross-sectional scanning tunneling microscopy and spectroscopy in order to achieve knowledge about its intrinsic electronic surface states. Atomically resolved STM images show a topographic contrast, which can be related with recent density functional theory calculations, and indicate a local charge enhancement within the surface unit cell. Scanning tunneling spectra reveil intrinsic states within the fundamental bulk band gap. Furthermore, the Fermi level is energetically located within the bulk band gap. This finding leads to the assumption that electron accumulation at this surface is not an intrinsic property, but related to extrinsic effects, such as e.g., non-stoichiometric material re-organization.

DS 30.9 Wed 17:45 POT 081

Electrical properties of In2O3 single crystals: distinction between surface and bulk conductivity — •Klaus Irmscher, Mike Pietsch, Wolfram Troeder, and Zbigniew Galazka — Leibniz-Institut für Kristallzüchtung, Berlin

Transparent semiconducting oxides such as In2O3, SnO2 or ZnO have the tendency to form surface electron accumulation layers. The highly conductive surface layers may have strong implications in the emerging field of transparent oxide electronics. For instance, the implementation of active elements like Schottky diodes depends on whether the accumulation of electrons at the surface can be suppressed in a controlled manner. Investigations on the origin of the surface electron accumulation in In2O3 were hitherto performed on thin crystalline films. Here, we present temperature dependent Hall effect measurements of melt-grown In2O3 bulk single crystals. The samples had electron concentrations between 10^16 and 10^19 cm-3 at room temperature depending on post-growth annealing conditions. The temperature dependent electron concentrations measured from 15 to 750 K show clear contributions due to surface electron accumulation. To differentiate between bulk and surface proportions the data evaluation is based on a two-layer model. This enables a clear attribution of donor concentration changes due to sample annealing under oxidizing or reducing conditions to surface-near and bulk regions, respectively. We discuss the possible influence of oxygen vacancies, hydrogen donors and surface adsorbates.

DS 30.10 Wed 18:00 POT 081

Electronic surface properties of stoichiometric and defect-rich indium oxide films prepared by MOCVD — •Marcel Himmerlich[1], Chunyu Wang[2], Volker Cimalla[2], Oliver Ambacher[2], and Stefan Krischok[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastraße 72, 79108 Freiburg, Germany

The influence of metalorganic chemical vapor deposition conditions on the indium oxide surface properties is investigated using photoelectron spectroscopy (PES). It is shown that the growth conditions have a strong influence on the physical properties and that films prepared at 200°C or below are highly oxygen-deficient and rich in defects, influencing the surface chemical and electronic properties and resulting in the existence of excess electrons, which are partially localized at the remaining indium atoms. This configuration results in the existence of reactive defect sites, which cause high ozone sensitivity. The PES results are compared to the electronic properties of crystalline In_2O_3 films in cubic bixbyite and rhombohedral structure. The influences of the surface stoichiometry and high defect density, ozone oxidation and UV photoreduction on variations in surface band bending, electron accumulation, work function and formed surface dipoles as well electron transport and sensor characteristics are analyzed.

DS 30.11 Wed 18:15 POT 081

Stability of low-index bcc-In_2O_3 surfaces under O-Rich-, In-Rich-, and Sn-doping molecular beam epitaxy conditions: An Experimental Study — •Oliver Bierwagen[1,2], Patrick Vogt[1], and James S. Speck[2] — [1]Paul-Drude-Institut, Berlin,Germany. — [2]University of California, Santa Barbara, USA.

Molecular beam epitaxy of bixbiyte In_2O_3 on (001) oriented ZrO_2:Y (YSZ) substrates typically results in {111} faceted surfaces whereas on (111) smooth films are obtained [1]. This behavior has been explained by theory calculations that found the surface free energies of low index bixbiyte surfaces to increase from (111) to (011) to (001) surfaces [2]. On the other hand, it was found that In-rich growth conditions [1] or high Sn-doping [6] lead to the formation of smooth, unfaceted (001) In_2O_3 films on YSZ(001). These results are in-line calculations of stoichiometry-dependent surface free energy [5]. Our experimental study of In_2O_3 on YSZ(001), (011), (111) grown by MBE under O-rich, In-rich and high Sn-doping conditions suggest the following relative surface free energies: (111) lowest under all conditions, (001) significantly lowered by In-rich conditions and Sn-doping. A flat (011) surface was not observed suggesting a higher surface free energy than predicted by theory. Our experimental results compare well to theory of [5]. [1] Bierwagen, Appl. Phys. Lett. 95, 262105 (2009). [2] Walsh and Catlow, J. Mater. Chem. 20, 10438 (2010). [4] Bierwagen and Speck, J. Appl. Phys. 107, 113519 (2010). [5] Agoston and Albe, Phys. Rev. B 84, 045311 (2011). [6] Taga, Jpn. J. Appl. Phys. 37, 6585 (1998).

DS 30.12 Wed 18:30 POT 081

Surface structure of metal oxides via classical and quantum mechanical rainbow scattering — •Marco Busch[1], Eric Meyer[1], Jan Seifert[1], Helmut Winter[1], Klaus Irmscher[2], and Zbigniew Galazka[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 and molecules with energies from 200 eV up to several tens of keV are grazingly scattered from clean and flat metal oxide surfaces. 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. As examples, we present investigations of the quantum scattering from the cleaved (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 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 thermal induced reconstruction of the $(11\bar{2}0)$ and (0001) surface of Al_2O_3 we found also a preservation of the longitudinal coherence and observed Laue circles of higher orders.