DS 28: Focussed Session: Oxide Semiconductors for Novel Devices I

Wide band gap semiconducting oxides such as the group-III sesquioxides find potential application in e.g. UV- or deep UV-sensors, transparent photovoltaic devices, power electronics or quantum well infrared photo detectors. This session sets a focus on growth of binary bulk material and thin films, the physical properties of these and their surface, properties of heterostructures and interfaces and the fabrication and performance of demonstrator devices.

Organizers: Oliver Bierwagen (PDI Berlin) and Holger von Wenckstern (U Leipzig)

Time: Wednesday 9:30–13:00 Location: CHE 89

Topical Talk DS 28.1 Wed 9:30 CHE 89

Self-consistent hybrid functional calculations: Electronic and optical properties of oxide semiconductors — •Daniel Fritsch[1], Benjamin Morgan[1], and Aron Walsh[1,2] — [1]Department of Chemistry, University of Bath, BA2 7AY Bath, UK — [2]Department of Materials, Imperial College London, SW7 2AZ London, UK

Owing to limitations of existing approximate exchange-correlation functionals, band gaps of semiconductors and insulators are often severely underestimated in density functional theory calculations. Considerable improvements are possible by including a fraction of Hartree-Fock exchange, constructing a so-called "hybrid" functional. The precise proportion of Hartree-Fock exchange is typically treated as an empirical parameter chosen from intuition and experimental calibration.

A recent self-consistent hybrid functional [1] removes this empiricism and offers a new approach for parameter-free hybrid functional investigations. Moreover, it provides a better starting point for many-body perturbation calculations based on the *GW* approximation. Applying this approach to a range of oxide semiconductors, we report on the electronic and optical properties, and compare them to other theoretical and experimental data [2].

[1] J. H. Skone, M. Govoni, and G. Galli, Phys. Rev. B **89**, 195112 (2014).
[2] D. Fritsch, B. Morgan, and A. Walsh, Nanoscale Research Letters **12**, 19 (2017).

DS 28.2 Wed 10:00 CHE 89

High-throughput screening of transparent conducting oxides — •Christopher Sutton[1], Robert J. N. Baldock[2], Luca M. Ghiringhelli[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Transparent conducting oxides (TCOs) are a well-developed and commercialized class of wide-bandgap semiconductors that are crucial for the function of many electronic devices. Recent experimental work has demonstrated bandgap engineering in ternary $(Al_xGa_yIn_z)_2O_3$ over 3 eV by adjusting the ratio of In/Ga and Ga/Al. The phase diagram for ternary and quaternary $(Al_xGa_yIn_z)_2O_3$ (where $x+y+z=2$) are examined using DFT-based cluster expansion models combined with fast stochastic optimization techniques (nested sampling) to efficiently search (meta)stable configurations for many different crystal structures. A new semi-grand-ensemble implementation enables exploration of ternary and quaternary $(Al_xGa_yIn_z)_2O_3$. With an extensive search over configurational space, statistical learning is performed for the bandgaps and stabilities to identify structure-property relationships between the targeted properties (e.g., optical transparency) and the fundamental chemical and physical parameters that control these properties.

DS 28.3 Wed 10:15 CHE 89

Pressure-dependent elastic properties of Ga_2O_3 in the α and β phase from first principles — •Konstantin Lion, Dmitrii Nabok, Pasquale Pavone, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin D-12489 Berlin

The structural and elastic properties of the monoclinic β and the hexagonal α phase of the transparent conducting oxide Ga_2O_3 are investigated from first principles using the full-potential all-electron code `exciting` [1]. The full stiffness tensor at fixed pressure of both phases is calculated using the tool `ElaStic` [2]. All eigenvalues of the stiffness tensor at zero pressure are positive and therefore both phases are considered elastically stable at equilibrium according to the Born stability criterion. The bulk moduli at $p = 0$ GPa for both phases, $B_0^\alpha = 218.48$ GPa and $B_0^\beta = 169.38$ GPa, are calculated as a linear combination of second-order elastic constants and show good agreement with previous results [3]. We also investigate the behavior of the stiffness tensor under load. The removal of band degeneracies and changes in the electronic band structure of both phases are investigated under the influence of different kinds of strain.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184**, 1861 (2013).
[3] J. Furthmüller *et al.*, Phys. Rev. B **93**, 115204 (2016).

DS 28.4 Wed 10:30 CHE 89

***Ab-initio* lattice dynamics of Ga_2O_3 polymorphs with an emphasis on polar phonon modes** — •Rut Waldenfels, Dmitrii Nabok, Pasquale Pavone, and Claudia Draxl — Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

Gallium oxide is a promising material for novel opto-electronic devices, due to its large band gap and its remarkable high carrier mobilities. Understanding electron-phonon interactions and in particular polaronic effects is essential for describing transport properties in polar materials. In this work, we perform a comparative study of the lattice dynamics of the two most stable polymorphs of Ga_2O_3, the α and β phase, using density-functional theory. We include non-analytical contributions to the dynamical matrix which allow for the full description of polar phonon modes. For these modes, we calculate the dependence of frequencies and eigenvectors on the wave-vector direction. We investigate which modes have the strongest impact on the electronic structure by calculating mode effective charges and average long-range coupling constants.

DS 28.5 Wed 10:45 CHE 89

Anisotropic thermal conductivity in Ga2O3 — •Mitdank Rüdiger[1], Handwerg Martin[1,3], Galazka Zbigniew[2], and Fischer Saskia F.[1] — [1]AG Novel Materials, Institut für Physik der Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2 , 12489 Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

The monoclinic crystal structure of β-Ga2O3 causes a significant anisotropy of the thermal properties. The temperature-dependent values of the thermal diffusivity D in [010] and [001] direction as well as thermal conductivity values λ in [100], [010] and [001] direction using Mg-doped insulating monoclinic β-Ga2O3 bulk crystals were measured by the 2-Omega-method [1,2]. The measurements were carried out by using the same sample. The room temperature values for the thermal conductivity in the main crystal axes are determined to λ[100] = 11+-1 W/(mK), λ[010] = 29+-2 W/(mK) and λ[001] = 21+-2 W/(mK). For the diffusivity we found D[100] = 3,7+-0,4 mm*/s, D[010] = 9,6+-0,5 mm*/s and D[001] = 7,1+-0,4 mm*/s. The anisotropy factor is the same and independent of temperature. We found D[010]/D[001] = λ[010]/λ[001] = 1,4+-1. The temperature dependence of the thermal diffusivity and conductivity is in accord with phonon-phonon-Umklapp-scattering for T > 150 K.

[1] Handwerg et al., SST 31, 125006 (2016) [2] A. T. Ramu and J. E. Bowers, Rev. Sci. Instr. 83 ,124903 (2012)

15 min. break.

Topical Talk DS 28.6 Wed 11:15 CHE 89

Exceptional Points in Oxide Bulk and Metamaterials — •Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, D-04103 Leipzig

The spectral dispersion of exceptional points (singular optic axes) is measured for (monoclinic and thus biaxial) β-Ga_2O_3 bulk material in

the absorption regime. Also we show that exceptional points exist in fully transparent, optically 'effectively' biaxial, anisotropic microcavities, fabricated using an uniaxial cavity material with its axis inclined to the Bragg mirror growth direction. Here the lack of time reversal symmetry is mediated by the mode broadening, i.e. the photon escape from the – in principle – open cavity system. As a consequence the eigenmodes are generally elliptically polarized, and completely circularly polarized eigenmodes are expected in certain directions. Via geometric and chemical composition design degrees of freedom, the spectral and angular position of these chiral modes can be rationally designed. Thus circularly polarized emission becomes possible without the use of spin injection or internal or external magnetic fields.

DS 28.7 Wed 11:45 CHE 89

Dielectric function and band structure of α Ga_2O_3 — •Martin Feneberg[1], Anderson Janotti[2], Maciej D. Neumann[3], Norbert Esser[3], Luis Artus[4], Ramon Cuscó[4], Tomohiro Yamaguchi[5], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke Universität Magdeburg — [2]University of Delaware — [3]Leibniz-Institut fur Analytische Wissenschaften - ISAS - e.V. — [4]ICTJA-CSIC, Barcelona — [5]Kogakuin University

Polytypes of gallium oxide are a very promising class of materials for electronic device applications. It is possible to stabilize α-Ga_2O_3 by mist chemical vapor deposition on sapphire substrates. However, the optical properties of this metastable corundum-like phase have not yet been investigated thoroughly. Spectroscopic ellipsometry at room temperature has been applied to determine the ordinary ($\varepsilon_\perp$) dielectric function of α-Ga_2O_3. This corresponds to an electric field direction perpendicular to the optical axis (0001), which is the growth direction of the thin (about 400nm) α-Ga_2O_3 films. A high energy spectral range up to 20eV has been investigated using synchrotron radiation. Several high-energy transitions have been resolved, which are consistent with ab-initio calculations of the dielectric function that include the solution of the Bethe-Salpeter equation, i.e. Coulomb interaction between electrons and holes. The calculations suggest that α-Ga_2O_3 is an indirect semiconductor with its valence band maximum between Γ and K points of the Brillouin zone. Strong direct absorption onsets at around 5.3 and 6.2eV are found, only slightly higher in energy than the predicted band gap.

Topical Talk DS 28.8 Wed 12:00 CHE 89

Kinetics and thermodynamcis of binary and ternary oxides during molecular beam epitaxy — •Patrick Vogt and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany

Group-III and IV oxide semiconductors such as Ga_2O_3, In_2O_3, and SnO_2 may be efficiently n-type doped and have generated much interest due to their wide band gaps, optical transparency in the visible, as well as deep ultra-violet (DUV) regime of light. Alloying binary to ternary systems, combines their properties depending on their metal (Me) concentration, facilitates band gap engineering, and enables the growth of heterostructures, for applications such as transparent electronics, power transistors, or DUV detectors.

This talk presents a comprehensive understanding of the reaction kinetics and thermodynamics of oxides grown by plasma-assisted molecular beam epitaxy (MBE). The defined growth surface chemistry during MBE makes it an ideal system for studying fundamental growth processes. Knowing the reaction behavior of materials allows the systematic manipulation of their crystal and electronic characteristics depending on all growth parameters. Semi-empirical macroscopic kinetic growth models are presented predicting the Me incorporation and desorption of the mentioned compounds. These models may be generalized for other oxide systems and give information about the underlying reaction mechanisms these compounds are based on.

The findings are qualitatively applicable to other growth techniques such as pulsed laser- and metal-organic vapor phase deposition.

DS 28.9 Wed 12:30 CHE 89

Tin Assisted Growth of ϵ-Ga_2O_3 on c-plane Sapphire — •Max Kracht[1], Alexander Karg[1], Jörg Schörmann[1], and Martin Eickhoff[1,2] — [1]I. Physikalisches Institut, Justus Liebig Universität, Gießen, Germany — [2]Institut für Festkörperpysik, Bremen,Germany

Gallium oxide can crystallize in different polymorphs. The most common phase β-Ga_2O_3 is a promising material for high power devices and has therefore been widely studied. Although most physical properties such as the large band gap ($\approx 5eV$) are expected to be comparable for the different polymorphs , high quality material is needed to study their characteristics in detail. For example theoretical studies predict a high spontaneous polarization in ϵ-Ga_2O_3 , which would allow the realization of heterostructures with a two dimensional electron gas with high sheet carrier densities . This work focuses on the growth of gallium oxide on c-plane Al_2O_3 by plasma assisted molecular beam epitaxy. In the metal-rich growth regime gallium sub-oxide Ga_2O, which evaporates at growth temperature, is formed. With the addition of a small tin flux (flux ratio Ga/Sn = 10000) we can suppress this sub-oxide-etching and expand the growth window to more metal-rich conditions. Under these conditions phase pure ϵ-Ga_2O_3 is formed. A growth model for this tin assisted growth mode is presented.

DS 28.10 Wed 12:45 CHE 89

Transport properties of the In_2O_3 surface electron accumulation layer — •Alexandra Papadogianni, Julius Rombach, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

In_2O_3 is a natively n-type transparent semiconducting oxide with unique properties attractive for several applications. Particularly interesting is its surface electron accumulation layer (SEAL), which enables gas-sensing applications. The SEAL electrical transport properties will be the main focus of this talk.
We study single-crystalline In_2O_3 thin films grown by plasma-assisted molecular beam epitaxy (PA-MBE) on insulating buffer layers achieved by doping with Ni as a new compensating acceptor, in order to remove potential interface conductance. This provides us with a model system of reduced complexity, with the electrical conductivity of these films essentially consisting of two parallel contributions: the bulk of the film and SEAL. To further modulate either the SEAL or the bulk in a targeted way and disentangle their contributions to the overall conductivity, we "turn off" the SEAL by an oxygen-plasma treatment and the bulk by Ni-doping. As a result, this enables us to study the temperature dependent transport properties of each individual conductive system.