HL 9: Focus Session: Oxide Semiconductors for Novel Devices II

Organizers: Holger Eisele (TU Berlin) and Holger von Wenckstern (Uni Leipzig)

Time: Monday 15:00–17:30 Location: H34

HL 9.1 Mon 15:00 H34

Tin-assisted PLD-growth of epitaxial κ-Ga_2O_3 thin films — •M. Kneiss[1], A. Hassa[1], D. Splith[1], C. Sturm[1], H. von Wenckstern[1], M. Lorenz[1], T. Schultz[2], N. Koch[2], and M. Grundmann[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik — [2]Humboldt Universität zu Berlin, Institut für Physik

Among the polymorphs of Ga_2O_3, the orthorhombic κ-phase features some outstanding properties. In contrast to the monoclinic β-modification, it is expected to possess a large spontaneous electrical polarization of 23 $\mu C/cm^2$ [1], while still exhibiting a high E_g of $\approx$ 5 eV [2]. Alloying with Al_2O_3 or In_2O_3 further enables band gap as well as polarization engineering, such that heterointerfaces can be utilized to localize high electron densities in a 2DEG. To create high quality heterostructures, epitaxial growth of κ-Ga_2O_3 with high crystalline quality and smooth surfaces is necessary. We show the growth of κ-Ga_2O_3 (001) with well-defined in-plane epitaxial relationships on Al_2O_3 (00.1), STO (111), YSZ (111) and MgO (111) substrates by pulsed laser deposition (PLD). A Sn-doped Ga_2O_3 PLD-target was used to catalyze the κ-phase [3]. The growth in this phase, epitaxial relationships and a high crystalline quality were verified by XRD, while AFM measurements reveal smooth surface morphology. We propose surfactant-mediated epitaxy as possible growth mechanism [4].

[1] M. B. Maccioni *et al.*, Appl. Phys. Expr. **9**, 041102 (2016)
[2] J. Furthmüller *et al.*, Phys. Rev. B **93**, 115204 (2016)
[3] M. Orita *et al.*, Thin Solid Films **411**, 134 (2017)
[4] M. Kneiß *et al.*, APL Materials, Accepted (2018)

HL 9.2 Mon 15:15 H34

Effective electron mass anisotropy in α-Ga_2O_3 — •Martin Feneberg[1], Jürgen Bläsing[1], Rüdiger Goldhahn[1], and Kazuaki Akaiwa[2] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg — [2]Department of Information and Electronics, Tottori University, Tottori 680-8552, Japan

Metastable α-Ga_2O_3 is a currently discussed candidate material system for future electronic devices. It is alloyable with corundum α-Al_2O_3 (sapphire) and α-In_2O_3. While p-type doping proves to be problematic, n-type doping by the substitutional donor tin is successful up to $n > 10^{19}$ cm^{-3}.

Here, we investigate the infrared optical properties of m-plane $(1\bar{1}00)$ α-Ga_2O_3 thin films grown on sapphire by mist chemical vapour epitaxy. Spectroscopic ellipsometry and Raman spectroscopy yields a full picture of the anisotropic phonon modes. A free-carrier contribution in degenerately highly doped material is found in the dielectric functions and yields anisotropic plasma frequencies.

By taking the Hall-effect free-electron concentration into account, effective electron masses of $m^*_\perp = 0.297 m_0$ and $m^*_{||} = 0.316 m_0$ are obtained at $n = 1.1 \times 10^{19}$ cm^{-3}. We finally discuss the nonparabolic dispersion relation of the conduction band rendering these values to be upper limits for the effective masses at the Γ-point of the Brillouin zone.

HL 9.3 Mon 15:30 H34

Transport Properties and Finite Size Effects in β-Ga_2O_3 Thin Films — •Robin Ahrling[1], Johannes Boy[1], Martin Handwerg[1], Olivio Chiatti[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], Günter Wagner[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, 12489 Germany

As a wide-band gap semiconductor with a high breakthrough field, gallium oxide (Ga_2O_3) has shown to be a promising material for applications in high power electronics. Here, we investigate the electrical properties of thin films and their dependence on film thickness. The scattering processes in the films may changes drastically with decreasing film thickness. [1]

Homoepitaxially MOVPE-grown monocrystalline Si-doped β-Ga_2O_3 films (28 - 225 nm thickness) were electrically characterized in a temperature range from 300 K down to 10 K. Van-der-Pauw and Hall-measurements were performed to determine conductivity, Hall density and carrier mobility. Thicker films (>150 nm) show a behavior similar to the bulk. Below 100 nm, a drastic drop of the mobility with decreasing thickness was observed, pointing to an additional surface scattering effect. We find that the commonly applied classical Fuchs-Sondheimer model does not explain the contribution of electron scattering at the film surfaces sufficiently. Instead, by applying an electron wave model by Bergmann, a mobility suppression due to the large de Broglie wavelength in β-Ga_2O_3 is proposed as a limiting quantum mechanical size effect. [1] R. Ahrling *et al.*, https://arxiv.org/abs/1808.00308

HL 9.4 Mon 15:45 H34

Properties of the β-Ga_2O_3(1 0 0) surface — •Jonathan K. Hofmann[1], Celina S. Schulze[1], Wjatscheslav Martyanov[1], Martin Franz[1], Zbigniew Galazka[2], and Holger Eisele[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Germany — [2]Leibniz-Institut für Kristallzüchtung, Germany

β-Ga_2O_3 is a wide band gap material showing n-type conductivity. The electrical conductivity of β-Ga_2O_3 can be controlled by growth environment, intentional doping, or post-growth heat treatment. Due to its large band gap of 4.85 eV, β-Ga_2O_3 is a promising material for high power electronics and UV optoelectronics.

The β-Ga_2O_3 single crystals were grown from the melt by the Czochralski method [1] and show good conductivity. For the present study, a sample was cleaved in UHV and the (1 0 0) surface was investigated with low energy electron diffraction (LEED) and scanning tunnelling microscopy/spectroscopy (STM/STS). The LEED-patterns show the unreconstructed (1 0 0) surface. STM images with atomic resolution display an atomically flat surface with dark contrasts. These dark contrasts are likely induced by oxygen vacancies below the surface. STS reveals an electronic state 1.5 eV below the conduction band minimum. This state is probably induced by the (+2/0) transition level of the oxygen vacancies.

The project was supported by the Leibniz Association, Leibniz Science Campus GraFOX, project C2-3.

[1] Z. Galazka et al., ECS J. Solid State Sci. Technol. **6**, Q3007 (2017).

HL 9.5 Mon 16:00 H34

Low-frequency noise characterization of MOCVD-grown β-Gallium Oxide — •Christian Golz[1], Günther Wagner[2], Andreas Popp[2], Fariba Hatami[1], and W. Ted Masselink[1] — [1]Department of Physics, Humboldt-Universität zu Berlin, Newton-Str. 15, D-12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Low-frequency noise spectroscopy was used to characterize β-Ga_2O_3 epilayers. These high-quality Si-doped layers were homoepitaxially grown by metal-organic chemical vapour deposition (MOCVD) on insulating Mg-doped β-Ga_2O_3 substrates. For noise measurements, Greek cross structures were processed using optical lithography. Hot H_3PO_4 etch was applied to process the mesa structures. Ohmic Cr/Au contacts were processed by thermal evaporation. Low-frequency noise is produced by the fluctuations in conductivity in a material. The 1/f noise intensity was used to determine a room temperature Hooge factor below 10^{-4}. This value indicates a high structural quality of the epilayer. Generation-recombination noise was analyzed between 80 K and 400 K. Several trap levels were found with characteristic time constants depending exponentially on temperature. Activation energies for these levels were determined to be in the range from 30 meV to 300 meV.

HL 9.6 Mon 16:15 H34

Ion beam Doped Transparent Conductive Oxides for Metasurfaces — •Alexander Koch, Jura Rensberg, Martin Hafermann, and Carsten Ronning — Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Transparent conductive oxides have recently gained a lot of attention for applications in plasmonics and nanophotonics due to their low optical loss, metal-like behavior, tailorable optical properties, and well established fabrication procedures. In particular, n-type doped zinc oxide (ZnO), such as aluminum doped ZnO (AZO), is very attractive because its dielectric permittivity can be precisely engineered over a broad range in the near-IR and IR regime via its doping level. Here,

we show that a very high doping concentration in ZnO can be achieved by ion implantation and post implantation annealing treatments. Furthermore, ion implantation offers the great opportunity of area selective doping using either focused ion beams or appropriate lithography techniques in combination with ion implantation. By this means, metasurfaces can be fabricated, which are composed of subwavelength sized structure elements possessing high optical contrast.

HL 9.7 Mon 16:30 H34

Phase transitions in Zn_2GeO_4: Insights from first-principles calculations — •Daniel Fritsch[1], Joachim Breternitz[1], and Susan Schorr[1,2] — [1]Department Structure and Dynamics of Energy Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Department of Geosciences, Freie Universität Berlin, Malteserstr. 74-100, 12249 Berlin, Germany

At ambient conditions, Zn_2GeO_4 crystallises in the thermodynamically stable willemite-type structure. However, under high-pressure, it is known to undergo a phase transition into a spinel-type phase. Given the plethora of possible applications for Zn_2GeO_4, ranging from cathode material in Li-ion batteries to photocatalyst system, requires a deeper understanding of the material properties in consideration of possible phase transitions.

Here, we will show results on the structural and electronic properties of Zn_2GeO_4 based on density functional theory calculations. Structural properties have been calculated using the PBEsol and the hybrid HSE06 functionals, and will be compared to results from a combined X-ray and neutron powder diffraction study. The electronic properties, e.g. band structure and effective masses, will be discussed as well.

This work made use of computational resources provided by the North-German Supercomputing Alliance (HLRN), and the Soroban and Dirac HPC facilities of the Freie Universität Berlin and the Helmholtz-Zentrum Berlin, respectively.

HL 9.8 Mon 16:45 H34

A theoretical study of Electronic and Optical Properties of Mercaptocarboxylic Acids on ZnO Surfaces — •Michael Lorke[1], Dennis Franke[1], Andreia daRosa[1,2], and Thomas Frauenheim[1] — [1]University of Bremen, Germany — [2]Institute of Physics, Federal University of Goiás,Brazil

In this work we investigate the electronic properties of mercaptocarboxylic acids with several carbon chain lengths adsorbed on ZnO-(10-10) surfaces via density functional theory calculations using semi-local and hybrid exchange-correlation functionals. Amongst the investigated structures, we identify the monodentate adsorption mode to be stable. Moreover, this mode introduces optically active states in the ZnO gap, is further confirmed by the calculation of the dielectric function at PBE0 and TD-PBE0 levels. One interesting finding is that adsorption mode and the dielectric properties of the hybrid system are both rather insensitive to the chain length, since the acceptor molecular state is very localized on the sulphur atom. This indicates that even small molecules can be used to stabilize ZnO surface and to enhance its functionality for opto-electronic applications.

HL 9.9 Mon 17:00 H34

Thermodynamics and electronic structure of low-index β-Ga_2O_3 surfaces — •Konstantin Lion[1,2], Sergey V. Levchenko[3,2,4], Matthias Scheffler[2], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Berlin, DE — [2]Fritz-Haber-Institut der MPG, Berlin, DE — [3]Skolkovo Innovation Center, Moscow, RU — [4]NUST MISIS, Moscow, RU

The surface properties of β-Ga_2O_3 play a vital role in epitaxial growth, electrical contacts, and gas sensors, but are still not well understood. In this work, we study the stability and electronic structure of several non-polar low-index surfaces of β-Ga_2O_3 using *ab initio* atomistic thermodynamics. Employing the efficient high-precision all-electron code FHI-aims, we perform density-functional-theory calculations with the HSE06 hybrid exchange-correlation functional. Numerous surface free energies are calculated, also including vibrational contributions. We find that the (100) surface is the most stable one, in agreement with previous reports [1], but, quite suprisingly, it is followed closely by the $(\bar{2}01)$ surface. Here, the topmost surface layers are significantly flattened upon relaxation, reducing the surface energy to 40 % of the value of the unrelaxed surface. This result explains recent experimental findings where $(\bar{2}01)$ facets were found to form during homoepitaxial growth on off-oriented β-Ga_2O_3 (100) substrates [2]. For this surface the electronic structure also reveals a strong surface resonance at the top of the valence band.

[1] V.M. Bermudez, Chem. Phys. **323**, 193 (2006).
[2] R. Schewski *et al.*, APL Materials **7** (2019), in print.

HL 9.10 Mon 17:15 H34

Nanostructured Metal-Oxides as Chemiresistive Gas Sensors for Breath Analysis — •Zafer Ziya Öztürk, Onur Alev, Neslihan Sarica, Alp Kiliç, and Serkan Büyükköse — Gebze Technical University, Çayirova Campus, 41400 Gebze/KOCAELI TURKEY

Recently, breath analysis has attracted much attention for disease monitoring and clinical diagnostics due to its non-invasive and therapeutic features. A number of breath markers or tracer compounds are summarized and related to different diseases, such as ammonia (kidney disease), HCN (bacterial infection), CO (lung inflammation), NO (asthma) and acetone (diabetes).

For point-of-care diagnosis, a portable, low cost and user-friendly sensors are desirable. To meet these requirements, emphasis is placed on metal-oxide (MOX) based chemiresistive gas sensors. Chemiresistive type sensors using various semiconducting MOXs, such as SnO2, ZnO and NiO have been considered for use as exhaled breath sensors due to their adequate reaction with volatile organic compounds. One dimensional nanostructures have attracted considerable interest due to their high surface-to-volume ratio and unique electrical properties. These features make them promising candidates for highly sensitive and selective breath analysis. In this work, nanostructured MOXs; ZnO, TiO2, CuO and WO3 sensors were fabricated by different techniques such as hydrothermal, electrochemical deposition and anodization. Fabricated sensor devices were tested towards some breath markers such as acetone, ammonia, HCN and ethanol in the range of ppb and sub-ppm.