DS 37: Focus Session: Functional Metal Oxides for Novel Applications and Devices II (joint session HL/DS)

Metal oxides exhibit a myriad of fascinating physical properties that enable a large variety of potential applications such as sensors and detectors, solar energy harvesting, transparent and potentially bendable electronics, power electronics, high-electron-mobility transisitors, memristors, topological quantum computation and so on. These functionalities typically require homo- or heteroepitaxial layers of high crystallinity with bendable amorphous semiconducting oxides as an exception. This session sets a focus on growth of bulk and thin films, experimental and theoretical investigation of their physical properties as well as fabrication and characterization of demonstrator devices.

Organizers: Oliver Bierwagen (Paul-Drude-Institut für Festkörperelektronik, Berlin), Holger Eisele (TU Berlin), Jutta Schwarzkopf (Leibniz-Institut für Kristallzüchtung, Berlin) and Holger von Wenckstern (Universität Leipzig).

Time: Thursday 9:30–13:00 Location: POT 81

Invited Talk DS 37.1 Thu 9:30 POT 81

Basics of Gas Sensing with Semiconducting Metal Oxides — •Nicolae Barsan — University of Tuebingen, Tuebingen, Germany

This contribution will present the basic knowledge needed to understand gas sensing with semiconducting metal oxides. It will explain how the interaction with atmospheric gases changes both surface charge and free charge carriers concentration and will descrice that in terms of reception and transduction functions. The body of essential data needed for the understanding of sensing for the case of two representative oxides, namely SnO2 and WO3 will be presented together with the description of the most relevant operando investigation techniques, namely Kelvin probe work function changes measurements and Diffuse Reflectance Infrared Fourier Transform Spectroscopy.The example of CO detection in the presence of humidity will be in the focus. It will be shown how this knowledge can be formalized with the help of the quasi-chemical reactions. Furthermore it will be explained how the charging of the surface changes the properties of the oxide and how this can be quantified with the help of the Poisson and electro-neutrality equations for both n and p-type materials.

DS 37.2 Thu 10:00 POT 81

Optical and photocatalytic properties of gallium-zinc-oxynitrides thin films grown by molecular beam epitaxy — •Elise Sirotti, Max Kraut, Florian Pantle, and Martin Stutzmann — Walter Schottky Institut and Physics Department, Technische Universität München, Am Coulomwall 4, 85748 Garching, Germany

GaN and ZnO are two well-studied materials with favorable energy positions of their band edges with respect to the redox levels of many electro-chemical reactions. However, their large band gap limits the use for simultaneous efficient solar light absorption and photocatalytic activity. By forming an alloy of both materials, the band gap can be reduced by more than 1 eV, while the energetic position of the conduction band stays almost constant. We present the growth of GZNO thin films by means of plasma-assisted MBE on c-plane sapphire. The quality and composition of the quaternary compound have been optimized by varying the temperature, metal fluxes and nitrogen-to-oxygen ratio during deposition. We performed photo-thermal deflection spectroscopy, valence band XPS and EDX measurements to investigate the influence of the composition on the electronic properties. As a result, the influence of the different components on the energetic positions of the conduction band and valence band has been clarified. With electrochemical measurements, we gain insights into the photo-catalytic activity and stability of the thin films. The high flexibility gained by MBE growth allows us to acquire additional knowledge about the fundamental principles of the band gap narrowing process.

DS 37.3 Thu 10:15 POT 81

Surface Stability of β-Ga_2O_3 at Realistic Temperature and Pressure Conditions from First Principles — •Konstantin Lion[1,2], Sergey V. Levchenko[3,2], Matthias Scheffler[2,1], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Berlin, DE — [2]Fritz-Haber-Institut der MPG, Berlin, DE — [3]Skolkovo Institute of Science and Technology, Moscow, RU

The surface properties of a material play a vital role in epitaxial growth and electrical contacts. Depending on the miscut direction on off-oriented (100) β-Ga_2O_3 substrates, homoepitaxially grown layers show distinct surface morphologies, i.e., the formation of $(\bar{2}01)$ facets [1]. In a first-principles approach, it is important to account for the experimental growth conditions, since they can influence surface stability and thus surface faceting. In this work, we study the stability of all symmetrically inequivalent low-index surfaces of β-Ga_2O_3 at realistic conditions using *ab initio* atomistic thermodynamics. In the calculation of the phase diagrams of all surfaces, we include vibrational contributions to the surface free energy. We find that $(\bar{2}01)$ faceting on (100) substrates is thermodynamically favored at $T = 825\,^{\circ}\mathrm{C}$ and an oxygen partial pressure of 1 mbar, the conditions during homoepitaxial growth. This shows that thermal equilibrium has been reached during growth. Also, we find that the (001) surface is stabilized at higher oxygen chemical potentials, which explains its role as a cleavage plane at ambient conditions.

[1] R. Schewski *et al.*, APL Materials **7**, 022515 (2019)

DS 37.4 Thu 10:30 POT 81

Investigations of β-Ga_2O_3(100) cleavage surfaces by scanning tunneling microscopy and spectroscopy — •Celina Seraphin Schulze[1], Jonathan Hofmann[1], Christian Bruckmann[1], Martin Franz[1], Zbigniew Galazka[2], Wjatscheslav Martyanov[1], and Holger Eisele[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany

We present surface investigations of three differently doped β-Ga_2O_3 crystals by scanning tunneling microscopy and spectroscopy. One sample is unintentionally doped, while both others are doped by Si and Sn. All the bulk β-Ga_2O_3 single crystals were grown from the melt by the Czochralski method [1,2] and cleaved *in situ* under a base pressure below 1×10^{-8} Pa for experimental investigation. On the flat β-Ga_2O_3(100) cleavage surfaces of each sample dark contrasts occur that can be partially assigned to unintentional background doping by Si. By low energy electron diffraction measurements on the β-Ga_2O_3(100) surfaces we observed an unreconstructed surface with a 1×1 diffraction pattern. Scanning tunneling spectra show intrinsic electronic states within the band gap, induced most likely by oxygen vacancies. This 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)

[2] Z. Galazka *et al.*, J. Crystal Growth 529, 125297 (2020)

DS 37.5 Thu 10:45 POT 81

Growth and characterization of Si delta-doped β-Ga_2O_3 layers by MOVPE — •Saud Bin Anooz, Raimund Grüneberg, Robert Schewski, Martin Albrecht, Andreas Fiedler, Klaus Irmscher, Zbigniew Galazka, Günter Wagner, and Andreas Popp — Leibniz-Institut für Kristallzüchtung (IKZ), Max-Born-Str. 2, 12489 Berlin, Germany

Si delta-doped β-Ga_2O_3 layers have been grown on (100) and (010) β-Ga_2O_3 substrates by MOVPE. AFM images of the grown layer on (010) oriented substrate show 2D island growth, while for layers grown on (100) with 6o miscut angle substrate step flow growth mode has been found resulting in a lower surface roughness for the (100) surface compared to (010). The amount of Si incorporated into the grown layers as well as the shape of the interface were studied by secondary ion mass spectrometry (SIMS). The SIMS depth profile for the Si delta-doped layer grown on a (010) substrate shows a gradual transition

from the high Si doped to the unintentionally doped regime. However, the Si depth profile of the layer grown on (100) 6° off substrate shows sharp interfaces between the high and low doped regions, a clear advantage with regard to later devices. This could be explained by the surface morphology of the grown layers on (010) and (100) substrates.

30 min. break

Invited Talk DS 37.6 Thu 11:30 POT 81

Ultra-thin oxides on InGaN nanowires: Passivation layers for nanostructured photoelectrodes and optical analysis of chemical processes — Paula Neuderth[2], Mariona Coll[3], Jörg Schörmann[2], Christian Reitz[6], Jordi Arbiol[4], Roland Marschall[5], and •Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Experimental Physics I Justus Liebig University Giessen Germany — [3]Institut de Ciencia de Materials de Barcelona ICMAB-CSIC, Spain — [4]ICREA Pg. Lluís Companys 23 08010 Barcelona, Spain — [5]Physical Chemistry III, University of Bayreuth, Germany — [6]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology, Germany

We demonstrate an experimental strategy for systematically assessing the influence of surface passivation layers on the photocatalytic properties of InGaN nanowire (NW) photoanodes by combining photocurrent analysis, photoluminescence spectroscopy and high resolution transmission electron microscopy. We apply this approach to separate the influence of different mechanisms recombination and transport processes of photogenerated carriers and to compare the effect of TiO2, CeO2 and Al2O3 coatings deposited by atomic layer deposition. Due to efficient charge transfer from the InGaN NW core a stable TiO2-covered photoanode with visible light excitation is realized. As a second application we demonstrate that due to the sensitivity of the InGaN NW photoluminescence to surface adsorbed oxygen the optical analysis of oxygen diffusion in ultrathin ceria coatings deposited by atomic layer deposition is possible.

DS 37.7 Thu 12:00 POT 81

Growth Window, Solubility Limit and Material Properties of κ-$(Al_xGa_{1-x})_2O_3$ PLD thin films — •A. Hassa[1], C. Wouters[2], M. Kneiss[1], P. Storm[1], H. von Wenckstern[1], D. Splith[1], C. Sturm[1], M. Albrecht[2], and M. Grundmann[1] — [1]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin, Germany

The orthorhombic polymorph of Ga_2O_3, namely κ, is of increasing interest because of its predicted large polarization of $23\,\mu C/cm^2$ [1] rendering it well suited for possible usage e.g. in HEMT's. The high bandgap of about 5 eV [2] can be enlarged by alloying with Al_2O_3 enabling such heterostructure-based devices. We present κ-$(Al_xGa_{1-x})_2O_3$ thin films grown on (00.1)Al_2O_3 by tin-assisted pulsed laser deposition (PLD) [2]. For some thin films a homogeneous target with a defined composition and for an 2 inch in diameter thin film a two-fold PLD target consisting of Ga_2O_3/Al_2O_3 semicircular segments were utilized to grow a sample with laterally continuous composition spread [3]. Al content, growth rates and the occurrence of single phase κ-$(Al_xGa_{1-x})_2O_3$ depends systematically on growth conditions. Further, we present the dependence of structural and optical properties on alloy composition. The maximum observed Al incorporation in the κ-phase was $x = 0.46$ with a bandgap of 5.85 eV.

[1] M. B. Maccioni *et al.*, Appl. Phys. Express 9, 04102 (2016).
[2] M. Kneiß *et al.*, APL Materials 7, 022516 (2019).
[3] H. von Wenckstern *et al.*, CrystEngComm 15, 10020 (2013).

DS 37.8 Thu 12:15 POT 81

Epitaxy of κ-$(Al,Ga)_2O_3$ heterostructures and superlattices by VCCS-PLD — •Philipp Storm[1], Max Kneiss[1], Thorsten Schultz[2], Daniel Splith[1], Holger von Wenckstern[1], Norbert Koch[2], Michael Lorenz[1], and Marius Grundmann[1] — [1]Universität Leipzig, Felix-Bloch Institut für Festkörperphysik — [2]Humboldt Universität zu Berlin, Institut für Physik

Ga_2O_3 is a wide band gap semiconductor with pronounced polymorphism. The thermodynamically stable and therefore most often investigated polymorph is the monoclinic β-phase. However, the metastable, orthorhombic κ-phase gained significant interest due to its high predicted spontaneous polarization of $23\,\mu C/cm^2$ [1]. Exploiting the polarization differences at κ-$Ga_2O_3/CaCO_3$ [2] or κ-Ga_2O_3/κ-$(Al,Ga)_2O_3$ heterointerfaces could allow for the formation of 2DEGs with high carrier densities, crucial for QWIP or HEMT devices. Nevertheless, only little is known about κ-$(Al,Ga)_2O_3$ heterostructures [3]. In this work, VCCS-PLD (vertical continuous composition spread pulsed laser deposition) [4] was utilized for the growth of κ-$(Al,Ga)_2O_3$ heterostructures and superlattices that were investigated regarding structural, morphological and optical properties to evaluate their potential for device applications.

[1] M. B. Maccioni *et al.* : Appl. Phys. Express 9, 041102 (2016)
[2] S. B. Cho *et al.* : Appl. Phys. Lett. 112, 162101 (2016)
[3] P. Storm *et al.* : APL Mater. 7, 111110 (2019)
[3] M. Kneiß *et al.* : ACS Comb. Sci. 20, 643 (2018)

DS 37.9 Thu 12:30 POT 81

Tin-assisted growth of κ-$(Al_xGa_{1-x})_2O_3/(In_xGa_{1-x})_2O_3$ superlattice heterostructures by pulsed laser deposition — •Max Kneiss, Philipp Storm, Anna Hassa, Daniel Splith, Chris Sturm, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik

The orthorhombic κ-phase of Ga_2O_3 possesses a similarly high bandgap of 5 eV as the thermodynamically stable β-phase, but further is expected to exhibit a high spontaneous electrical polarization of $23\,\mu C/cm^2$ [1]. Polarization differences at interfaces of κ-phase heterostructures can be utilized for polarization doping to localize a 2DEG that typically features large carrier densities as well as high mobility. We present the coherent growth of κ-$(Al_xGa_{1-x})_2O_3/(In_xGa_{1-x})_2O_3$ quantum-well (QW) superlattices on c-sapphire substrates by pulsed laser deposition. Tin containing targets were necessary for the stabilization of the orthorhombic phase [2]. We found narrow superlattice oscillations up to the ninth order and up to $x \approx 0.5$ in XRD 2θ-ω scans as well as in reciprocal space maps for up to 15 layer pair superlattices confirming excellent crystal quality and abrupt interfaces. The evolution of superlattice oscillations as well as the optical properties will be evaluated in dependence on the QW and barrier width as well as on the composition of the QW and barrier layers. AFM measurements confirm smooth surface morphology for all samples. [1] Maccioni *et al.*, Appl. Phys. Expr. **9**, 041102 (2016) [2] Kneiß *et al.*, APL Materials **7**, 022516 (2019)

DS 37.10 Thu 12:45 POT 81

Band offsets at κ-$([Al,In]_xGa_{1-x})_2O_3/MgO$ interfaces — •Thorsten Schultz[1,2], Max Kneiss[3], Philipp Storm[3], Daniel Splith[3], Holger von Wenckstern[3], Marius Grundmann[3], and Norbert Koch[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany — [2]Helmholtz-Zentrum für Energie und Materialien GmbH, Berlin, Germany — [3]Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Leipzig, Germany

Conduction and valence band offsets are amongst the most crucial material parameters for semiconductor heterostructure device design. Due to its expected high spontaneous electrical polarization and the possibility of polarization doping at heterointerfaces, the metastable orthorhombic κ-phase of Ga_2O_3 and its indium and aluminum alloy systems are an interesting material class. We report on valence and conduction band offsets of κ-$(Al_xGa_{1-x})_2O_3$ and κ-$(In_xGa_{1-x})_2O_3$ thin films to MgO as reference dielectric by X-ray photoelectron spectroscopy. The determined band alignments reveal the formation of a type I heterojunction to MgO for all compositions with conduction band offsets of at least 1.4 eV, providing excellent electron confinement. We further found that the conduction band offsets in the alloy system are mainly determined by the evolution of the bandgaps. Therefore, tunable conduction band offsets of up to 1.1 eV within the alloy system allow for subniveau transition energies in corresponding quantum wells from the IR to the visible regime, which are promising for application in, e.g., quantum-well infrared photodetectors.