HL 25: Oxide Semiconductors I

Time: Wednesday 9:30–12:45 Location: ER 325

HL 25.1 Wed 9:30 ER 325

Photoluminescence study of corundum-like α-Ga_2O_3 — •Lennart Hölzer[1], Elias Kluth[1], Rüdiger Goldhahn[1], Dae-Woo Jeon[2], Kazuaki Akaiwa[3], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Korean Institute of Ceramic Engineering and Technology, Jinju, South Korea — [3]Department of Information and Electronics Engineering, Tottori University, Japan

Ga_2O_3 is a polymorphic ultra-wide band gap semiconductor with promising usage in power electronic devices like MOSFETs and Schottky diodes. Due to its thermodynamical stability, research has primarily focused on the stable β-phase.

Despite being metastable, α-Ga_2O_3 is just as interesting with an even wider band gap of ≈ 5.6 eV. Band gap engineering also has been proven possible in a range of about 3.7 to 9 eV by alloying with Al, In or Ti. This enables applications in devices such as solarblind photodetectors and FETs.

There is, nevertheless, a significant lack of knowledge of the optical properties. To investigate these, c-plane and m-plane α-Ga_2O_3 samples grown on sapphire substrates by HVPE and mist-CVD were studied using low temperature photoluminescence. A luminescence band in the UV-region at 3.75 eV was identified. The correlation of temperature and luminescence intensity was evaluated, yielding activation energies in the magnitude of the donor binding energy.

HL 25.2 Wed 9:45 ER 325

Red shift of the absorption onset in orthorhombic κ-$(In_xGa_{1-x})_2O_3$ alloys — •Elias Kluth[1], Alexander Karg[2], Martin Eickhoff[2], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Institut für Festkörperphysik, Universität Bremen, Germany

The polymorphic ultra-wide band gap semiconductor Ga_2O_3 is of high research interest as it offers potential in power electronics like MOSFETs, MeSFETs or Schottky diodes as well as in solar-blind UV detectors, and many more.

While previous research has mostly focused on the stable β- or the metastable α-phase, the orthorhombic κ-Ga_2O_3 is only poorly explored. This phase is predicted to be polar with a high spontaneous polarisation, potentially even higher than GaN, making it interesting for applications such as high electron-mobility transistors (HEMTs). Alloying κ-Ga_2O_3 with indium further extends these possibilities. For a successful device implementation, an understanding of the optical properties is essential.

Here, spectroscopic ellipsometry in the visible-ultraviolet range is perfomed on κ-$(In_xGa_{1-x})_2O_3$ with $x \leq 0.16$, grown by MBE (molecular beam epitaxy) on c-plane sapphire substrates, to obtain the complex dielectric function. An evaluation of the dielectric function yields a strong red shift in the absorption onset with increasing indium content (x).

HL 25.3 Wed 10:00 ER 325

Comparative study of temperature-dependent bandgap transitions in Ga_2O_3 polymorphs — •Benjamin M. Janzen[1], Nima Hajizadeh[1], Moritz Meissner[1], Marcella N. Marggraf[1], Conrad V. Hartung[1], Alwin Wüthrich[1], Nils Bernhardt[1], Felix Nippert[1], and Markus R. Wagner[2] — [1]Technische Universität Berlin — [2]Paul-Drude-Institut für Festkörperelektronik

The temperature dependence of the optical bandgap has rarely been investigated experimentally for the different polymorphs of Ga_2O_3. A direct comparison of the temperature dependence as well as the electron-phonon coupling strengths is made considerably more difficult by the different experimental methods (e.g., reflection spectroscopy, absorption spectroscopy or ellipsometry) used to study the various polymorphs. In particular, there is no study in the literature that provides a self-consistent comparison between the band gap values, the averaged phonon energies and the electron-phonon coupling strengths of the different polymorphs using the same experimental technique. We provide an experimental study to investigate the electronic bandgap transitions in monoclinic $\beta-$, orthorhombic $\kappa-$, rhombohedral $\alpha-$, defective-spinel γ- and cubic bixbyite $\delta-Ga_2O_3$ as a function of the sample temperature. Temperature-dependent UV photoluminescence excitation (PLE) spectroscopy is employed in the temperature range between 5 K and 300 K and the temperature dependencies are discussed regarding the energy bandgap, the effects of electron-phonon coupling and the averaged phonon energies.

HL 25.4 Wed 10:15 ER 325

Optical phonon modes in $LaInO_3$: Lattice dynamics and complete polarization analysis of Raman-active modes — •Hans Tornatzy[1], Roland Gillen[2], Zbigniew Galazka[3], Oliver Brandt[1], Manfred Ramsteiner[1], and Markus R. Wagner[1] — [1]Paul-Drude-Institut, Berlin — [2]Friedrich-Alexander Universität Erlangen-Nürnberg — [3]Leibniz-Institut für Kristallzüchtung, Berlin

$LaInO_3$ is part of the family of ABO_3 perovskites, and is considered promising for next generation devices such as for power electronics due to its band gap of about 4.5 eV. A detailed knowledge of phonon modes in $LaInO_3$ is important as they determine a number of material properties such as the mechanical and elastic properties, thermal transport and carrier dynamics, phonon-assisted optical excitations, and many more. However, little is known about the vibrational properties of this material. In this study, we investigate the lattice dynamics by polarization- and angle-resolved Raman spectroscopy and density functional theory (DFT). We experimentally observe all but one of the Raman active modes and compare them to our simulated values from DFT. Furthermore, we derive the phonon dispersion relation along the high symmetry directions in reciprocal space and depict the oscillation patterns for selected phonons at the Γ point. Finally, we determine the relative Raman tensor elements of the observed modes from the angular dependence of their corresponding scattering efficiencies.

HL 25.5 Wed 10:30 ER 325

Raman active phonon modes of single-domain orthorhombic κ-Ga_2O_3 — •Alwin Wüthrich[1], Benjamin M. Janzen[1], Hiroyuki Nishinaka[2], Roland Gillen[3], and Markus R. Wagner[1,4] — [1]Technische Universität Berlin — [2]Kyoto Institute of Technology — [3]Friedrich-Alexander Universität Erlangen-Nürnberg — [4]Paul-Drude-Institut für Festkörperelektronik, Berlin

Next-generation electronic and photonic devices require advanced materials with tailored properties. The orthorhombic κ-phase of Ga_2O_3 features an ultrawide bandgap around 5 eV, a large spontaneous polarization along the c-axis and ferroelectric behaviour. A major obstacle for device applications based on κ-Ga_2O_3 is the formation of rotational domains. Established growth techniques like MBE, MOVPE, PLD and mist CVD have so far only produced rotational-domain samples, where orthorhombic domains with sizes up to 200 nm align along three preferential directions that are 120°-rotated with respect to each other. Most recently, the growth of single-domain κ-Ga_2O_3 on orthorhombic ε-$GaFeO_3$ was demonstrated by mist CVD, resulting in a lattice mismatch as low as 1%. We present comprehensive Raman spectra of single-domain κ-Ga_2O_3, using a set of dedicated polarization geometries to resolve more than 100 of the 117 optical Raman-active modes experimentally. Moreover, we present the angular dependent Raman scattering intensities for excitation of the c-plane, proving the single-domain orthorhombic nature of the investigated thin film.

HL 25.6 Wed 10:45 ER 325

Determination of self-trapped exciton emission bands in Ga_2O_3 polymorphs — •Nima Hajizadeh[1], Benjamin M. Janzen[1], Moritz Meissner[1], Marcella N. Marggraf[1], Conrad V. Hartung[1], Alwin Wüthrich[1], Nils Bernhardt[1], Felix Nippert[1], and Markus R. Wagner[2,1] — [1]Technische Universität Berlin, Institute of Solid State Physics — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V.

Several temperature and excitation dependent photoluminescence (PL) and excitation (PLE) spectra are published for the thermodynamically stable β phase. In addition, a large number of theoretical calculations allow the assignment of observed emission bands. Accordingly, the UV bands in β-Ga_2O_3 are associated with the recombination of a self trapped hole (STH) and bound electrons. Such clear experimental assignments of optical bands for the different Ga_2O_3 polymorphs do not yet exist. Using temperature-dependent PL and PLE spectroscopy, we provide a study to investigate emission bands of monoclinic β-, orthorhombic κ-, rhombohedral α-, defective-spinel γ- and cubic bixbyite

δ-Ga_2O_3 as a function of excitation and temperature. Based on these spectra, a possible experimental identification of STH emission bands for different Ga_2O_3 polymorphs will be discussed. Furthermore, this evaluation may be supported by a correlation between the experimental stokeshifts and the theoretically calculated self-trapping energies in the literature, which would allow the detection and energetic determination of these excitons.

30 min. break

HL 25.7 Wed 11:30 ER 325

Nonlinear bond length change in zincblende Cu(Br,I) alloys — •Sandra Montag[1], Stefan Merker[2], Michael Bar[1], Richard J. Schenk[1], Eva Zollner[1], Konrad Ritter[1], Timo Pfeiffelmann[1], Sergiu Levcenko[1], Edmund Welter[3], Holger von Wenckstern[1], Marius Grundmann[1], Harald Krautscheid[2], and Claudia S. Schnohr[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Germany — [2]Institute of Inorganic Chemistry, Leipzig University, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

CuI is one of the most promising transparent p-type semiconductors with various applications from diodes to solar cells, including also flexible electronics [1]. Among numerous doping and alloying attempts, anion substitution with bromide can be used to tailor the free hole concentration in functional layers enabling optimized performance of active devices such as pn-diodes or transistors [2]. Using X-ray absorption spectroscopy, the element-specific fine structure of $CuBr_{1-x}I_x$ powder and thin film samples with anion composition x varying from 0 to 1 was measured. The near edge region is used to identify the presence and amount of oxygen contamination of the samples. The analysis of the extended fine structure reveals a nonlinear change of the Cu-Br and Cu-I bond lengths with composition x. This behaviour is different from that observed for III-V and II-VI zincblende alloys [3].

[1] Grundmann et al., *Phys. Status Solidi A* **210**, No. 9, 1671 (2013)
[2] Yamada et al., *Adv. Funct. Mater.* **30**, 2003096 (2020)
[3] Schnohr, *Appl. Phys. Rev.* **2**, 031304 (2015)

HL 25.8 Wed 11:45 ER 325

Magnetostriction in spinel zinc ferrite revisited: A first-principles investigation — •Daniel Fritsch — Zuse Institute Berlin, Takustr. 7, 14195 Berlin, Germany

Magnetostriction describes the property of materials to change its length or volume when going from randomly oriented magnetic moments to an ordered state by placing it in a magnetic field. Typically, these changes are of the order 10^{-6} or less, however, some materials have been shown to show larger magnetostriction, and have consequently been employed for sensor applications.

Among the material class of spinel ferrites, $CoFe_2O_4$ shows very large magnetostriction [1], and a recent experimental investigation reported similar in $ZnFe_2O_4$. Here, we revisit magnetostriction in $ZnFe_2O_4$ by means of first-principles calculations, employing density functional theory and hybrid exchange and correlation functionals [2], together with a recently devised method to speed-up these calculations [3]. The obtained results will be discussed with respect to available experimental findings and complement our knowledge about magnetostriction in spinel ferrites.

[1] D. Fritsch and C. Ederer, Phys Rev B **82**, 104117 (2010), Phys. Rev. B **86**, 014406 (2012).
[2] D. Fritsch, J. Phys.: Condens. Matter **30**, 095502 (2018).
[3] D. Fritsch, Appl. Sci. **12**, 2576 (2022).

HL 25.9 Wed 12:00 ER 325

Screening of contact metals for optimized performance of α-Ga_2O_3 based Schottky Barrier Diodes — •Sebastian Köpp, Clemens Petersen, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

We present α-Ga_2O_3:Sn based Schottky barrier diodes with exceptional current rectification ratios of up to 8 orders of magnitude and high mean barrier heights of up to 2.53 eV. By evaluating various Schottky metals, we find that reactively sputtered Pt/PtO_x yields the best performing Schottky barrier diodes [1]. We further show temperature dependent IV-measurements in the range of 40 K-400 K that are in agreement with the thermionic emission model. The effective barrier heights could accurately be fitted using the laterally inhomogeneous barrier model [2].
In recent years the metastable corundum-structured α-phase of Ga_2O_3 has shown to have promising physical properties. With a bandgap of 5.3-5.6 eV [3,4] and a predicted breakdown field of 10 MV/cm it surpasses the theoretical limits of β-Ga_2O_3 in terms of Baliga's figure of merit [4]. Further, α-Ga_2O_3 is isostructural to α-Al_2O_3 and hence epitaxial growth on cost-efficient sapphire substrates is feasible.

[1] S. Koepp *et al.*, J. Vac. Sci. Technol. A 41, 043411 (2023)
[2] D. Splith *et al.*, Phys. Status Solidi A, 218: 2100121 (2021)
[3] A. Segura *et al.*, Phys. Rev. Materials 1, 024604 (2017)
[4] E. Ahmadi *et al.*, J. Appl. Phys. 126, 160901 (2019)

HL 25.10 Wed 12:15 ER 325

Tailoring analog $TiN/SiO_x/Cu/SiO_x/TiN$ memristive devices through experiments and simulations — •Rouven Lamprecht[1], Tobias Gergs[2], Luca Vialetto[2], Finn Zahari[1], Richard Marquardt[1], Jan Trieschmann[2], and Hermann Kohlstedt[1] — [1]Chair of Nanoelectronics, Institute of Electrical and Information Engineering, Faculty of Engineering, Kiel University, Germany — [2]Chair of Theoretical Electrical Engineering, Institute of Electrical and Information Engineering, Faculty of Engineering, Kiel University, Germany

Memristive devices for neuromorphic circuits are an emerging nanotechnology promising for bioinspired computing architectures. Due to their voltage-dependent change in resistance, memristive devices can be considered as electronic pendants to synapses in the nervous system. In this study, we combine an experimental and modeling approach to systematically characterize the electrical properties of memristive devices, which were fabricated using different process methods with varying parameters. Experimental data provides local measurements of current-voltage (I-V) characteristics demonstrating analog switching of the $TiN/SiO_x/Cu/SiO_x/TiN$ memristive devices. Monte Carlo simulations provide insights into the fabrication conditions by modeling the deposition source (thermal evaporation and magnetron sputtering) as well as the deposited thin film composition. As a result of the study, we correlate the measured electrical device properties with simulated deposition properties to provide insights into the key operational conditions influencing the memristive behavior.

HL 25.11 Wed 12:30 ER 325

Two-dimensional electron gas in polar-discontinuity doped $LaInO_3/BaSnO_3$ heterostructure grown by plasma-assisted molecular beam epitaxy — •Georg Hoffmann[1], Martina Zupancic[2], Martin Albrecht[2], and Oliver Bierwagen[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

Transparent semiconducting oxides (TSO's) are key players for new (opto-)electronic devices. In the search for suitable TSOs, the wide-bandgap semiconductor $BaSnO_3$ has been reported to provide the highest room temperature electron mobilities within the perovskite oxides - up to 320 cm^2/Vs for La doped bulk material [1]. Interfacing the undoped, nonpolar $BaSnO_3$ with the closely lattice-matched, polar $LaInO_3$ is predicted to create a two-dimensional electron gas (2DEG) with a charge carrier density of up to $2\times10^{14}/cm^2$ due to polar-discontinuity doping [2]. Here, we demonstrate the adsorption-controlled growth of $LaInO_3/BaSnO_3$ heterostructures grown by plasma-assisted molecular beam epitaxy. The formation of the 2DEG at the $LaInO_3/BaSnO_3$ interface is confirmed by capacitance-voltage and van der Pauw-Hall measurements. The extracted sheet electron concentrations above $2\times10^{13}/cm^2$ and RT electron mobilities above 100 cm^2/Vs pave the way for further device studies.

[1] H. J. Kim et al., Appl. Phys. Express, 5, 061102 (2012). [2] K. Krishnaswamy et al., Appl. Phys. Lett. 108, 083501 (2016).