DS 42: Focus Session: Functional Metal Oxides for Novel Applications and Devices III (joint session HL/DS)

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 15:00–16:30 Location: POT 81

DS 42.1 Thu 15:00 POT 81

Ab-initio investigation of first-order Raman scattering in gallium oxide — •Rouven Koch, Pasquale Pavone, Dmitrii Nabok, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany

In this work, we investigate the Raman tensors and first-order spectra of the β and α phase of Ga_2O_3 by means of first-principles calculations using the *ab-initio* methodology implemented in the software package `exciting` [1]. We start from the determination of the equilibrium crystal structure of both polymorphs. Then, we explore the lattice dynamics of the two phases, paying special attention to the characterization of the phonons at the Γ point. The peculiar properties of the polar phonon modes of the β phase are addressed, including the LO-TO splitting and reflectivity spectra. Then, we compute the frequency-dependent dielectric tensors within the random-phase approximation. The lattice-dynamical properties and the dielectric tensors are used for the calculation of the Raman spectra in different polarizations. The obtained polarized Raman spectra for α- and β-Ga_2O_3 are compared to available data in the literature [2]. Our results highlight the fact that excitonic effects do not play a significant role on off-resonance Raman spectra. The overall good agreement with the experiments indicates the accuracy of the approximations used in this calculation.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202;

[2] C. Kranert *et al.*, Scientific Reports **6** (2016) 35964.

DS 42.2 Thu 15:15 POT 81

Raman-Spectroscopy of corundum-like α-Ga_2O_3 grown by HVPE — •Jona Grümbel[1], Pingfan Ning[1,3], Jürgen Bläsing[1], Dae-Woo Jeon[2], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität Magdeburg — [2]Korean Institute of ceramic Engineering and Technology, Seoul, South Korea — [3]School of Electronics and Information Engineering, Tiangong University, China

Ga_2O_3 is a high-bandgap semiconductor, whose stable β-phase is already applicable to semiconductor power devices like FETs and Schottky-Diodes. The metastable, corundum-like α-phase is less discussed, but allows bandgap-engineering by alloying with α-Al_2O_3 (sapphire) or α-In_2O_3.

Here, we investigate the lattice vibrations in the context of crystal quality. Therefore, three different samples grown by three different variations of HVPE (halide vapor phase epitaxy) are investigated. For the characterization of phonon modes, Raman Spectroscopy is employed.

All seven Raman-active phonon modes are identified in different Raman setup configurations. We investigate the correlation of phonon energies and lattice parameters as determined by x-ray diffraction. A small but detectable influence of phonon deformation potentials is found. Moreover, we find a very pronounced influence of crystal quality - as witnessed by ω-scan relative amplitudes - on certain Raman-active phonon modes which might be used as marker for ample quality.

DS 42.3 Thu 15:30 POT 81

Raman spectroscopy as a tool to determine the Néel temperature of NiO thin films in correlation with their structural characteristics — •Johannes Feldl, Melanie Budde, Carsten Tschammer, Oliver Bierwagen, and Manfred Ramsteiner — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5–7, 10117 Berlin, Germany

NiO is one of the most common natural antiferromagnetic (AF) oxides and a transparent p-type semiconductor making this material interesting for both, applications in the fields of spintronics and transparent-oxide electronics. One of the crucial magnetic parameters of AF materials is the Néel temperature (T_N). For thin epitaxial films of NiO, T_N will depend on the growth conditions and their resulting structural properties and is therefore expected to deviate from the value of 523 K for bulk NiO. Here, we utilize Raman spectroscopy to study the magnetic and structural properties of NiO thin films. The films are grown on MgO(100) substrates by plasma-assisted molecular beam epitaxy at different substrate temperatures. For the assessment of the structural properties, Raman scattering by optical phonons is analysed. Regarding the experimental determination of T_N, we demonstrate a reliable approach by analyzing the temperature dependence of the two-magnon (2M) peak in the Raman spectra. The obtained T_N values are below 480 K and are found to be correlated with the in-plane strain and the degree of lattice disorder in the NiO films.

DS 42.4 Thu 15:45 POT 81

Phonons and free-carrier contributions of spinel $ZnGa_2O_4$ by spectroscopic ellipsometry — •Alwin Wüthrich[1], Martin Feneberg[1], Zbigniew Galazka[2], and Rüdiger Goldhahn[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Leibniz Institute for Crystal Growth, Berlin, Germany

Ga based spinels with the general formula of $MeGa_2O_4$, where Me is a divalent metal, such as $MgGa_2O_4$ or $ZnGa_2O_4$ offer an ultra wide band gap and good electrical conductivity. These transparent semiconducting oxides (TSOs) have been receiving greater interest in the last years due to an outstanding importance in a wide range of scientific disciplines, such as photoelectronics, sensing systems or optical applications. Here, bulk $ZnGa_2O_4$ single crystals were grown directly from the melt by the vertical gradient freeze (VGF) method. This study presents a characterisation of these bulk crystals by spectroscopic ellipsometry, from which the complex dielectric function (DF) was deduced. Free-carrier concentrations (n) up to 10^{19} cm^{-3} were investigated in the infrared spectral range, where the phonons and plasmons were determined. The former agrees well to prior theoretical and experimental studies while from the latter the dependence of the effective electron mass on n is achieved, indicating a non-parabolicity of the conductive band.

DS 42.5 Thu 16:00 POT 81

Electric and Thermoelectric Properties of $ZnGa_2O_4$ Bulk Crystals — •Johannes Boy[1], Martin Handwerg[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Strasse 2, 12489 Berlin, Germany

In the past years, intense research has been done in the field of oxide semiconductor materials, which are promising candidates for the design of novel high power devices, optoelectronics and sensing systems due to their wide bandgap. $ZnGa_2O_4$ is a transparent material of blue coloration, with a high bandgap E_g=4.6 eV at room temperature [1]. The majority charge carrier type is n-type. Electron mobilities up to 100 cm^2/Vs with charge carrier concentrations in the order of 10^{18} - 10^{19} cm^{-3} have been reported [1]. In this work, we manufactured microlabs on the chip [2] to investigate the temperature dependence of the Seebeck coefficient S, Hall charge carrier density n and mobility μ between T = 10 K and T = 320 K. At high bath temperatures $T > 230K$, the scattering is determined by electron-phonon-interaction. At low bath temperatures (between 10 and 150

K) we observe a temperature-independent maximum, which can be explained by electrons interacting with ionized impurities. The room temperature Seebeck coefficient is $S_{(300K)} = (-120 \pm 3)\ \mu V/K$ and decreases with decreasing bath temperature.[1] Z. Galazka, *et al.*; APL Materials **7**, 022512 (2019).
[2] J. Boy, *et al.*; APL Materials **7**, 022526 (2019).

DS 42.6 Thu 16:15 POT 81

Low-frequency noise characterization of MOCVD-grown β-Gallium Oxide — •Christian Golz[1], Günter Wagner[2], Saud Bin Anooz[2], Zbigniew Galazka[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 defects and trap states in β-Ga_2O_3 epilayers. These high-quality Si-doped layers were homoepitaxially grown by metal-organic chemical vapour deposition (MOCVD)[1] on insulating Mg-doped β-Ga_2O_3 substrates prepared from bulk crystals obtained by the Czochralski method [2].

For noise measurements, lithographically defined Greek cross mesa structures were etched using hot H_3PO_4. Ohmic Ti/Au contacts were processed by e-beam evaporation. Generation-recombination noise, thermal noise, and 1/f noise are well resolved. Measured Hooge parameter values between 10^{-5} and 10^{-3} indicate a high structural quality of the epilayer. Generation-recombination noise was analyzed between 80 K and 400 K, finding up to three deep trap levels. Each of these deep traps is characterized in terms of their density, thermal activation energy, capture cross section prefactor, and binding energy.

[1] R. Schewski et al., APL Mater. 7, 022515 (2019); [2] Z. Galazka et al., ECS J. Solid State Sci. Technol. 6, Q3007 (2017)