HL 41: Oxide Semiconductors I: Ga_2O_3

Time: Thursday 15:00–17:00 Location: POT 81

HL 41.1 Thu 15:00 POT 81

Thermal Conductivities of Ga_2O_3 Polymorphs: Analysis of Anharmonicity and Anisotropy — •Shuo Zhao, Matthias Scheffler, and Christian Carbogno — The NOMAD Laboratory at the FHI of the Max-Planck-Gesellschaft and IRIS-Adlershof of the Humboldt-Universität zu Berlin

Gallium oxide (Ga_2O_3) is an ultra-wide bandgap material with substantial potential for electronics, e.g., in field effect transistors [1]. In this context, an atomistic understanding of its heat transport characteristics is essential for thermal management. For this purpose, we compute the lattice thermal conductivity of the α-, β-, and κ-polymorphs of Ga_2O_3 using the *ab initio* Green-Kubo formalism [2,3] that incorporates all orders of anharmonic effects via first-principle molecular dynamics. We discuss the role of anharmonic effects for the different polymorphs and investigate their influence on the anisotropy of the conductivity tensor. Our results provide guiding rules for maximizing and minimizing thermal transport in thin Ga_2O_3 films.

[1] M. Higashiwaki, *et al.*, *Appl. Phys. Lett.* **100**, 013504 (2012).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).
[3] F. Knoop, M. Scheffler, and C. Carbogno, *arXiv:*2209.01139 (2022).

HL 41.2 Thu 15:15 POT 81

Strain-induced polymorph conversion in gallium oxide via focused ion beam irradiation — •Umutcan Bektas, Paul Chekhonin, and Gregor Hlawacek — Insitute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Monoclinic β-Ga_2O_3 is chemically and thermally the most stable compound compared to its other polymorphs. It is a promising semiconductor material for power electronics, optoelectronics, and batteries. However, controlling the metastable polymorph phases is challenging, and the fabrication technology at the nanoscale is immature. Our goal is to understand and control the polymorph conversion, so we can establish new fabrication methods of single-phase polymorph coatings, buried layers, multilayers, and different nanostructures in gallium oxide.

Under ion beam irradiation, most semiconductors show transformation from crystalline to amorphous structure due to ion beam induced damage. However, it is observed that, this transformation is suppressed in gallium oxide, and a polymorph conversion is observed instead. Here, we use Gallium and Neon focused ion beams (FIB) from different sources (GFIS, LMIS) to create local strain and induce the polymorph transition. After irradiation, characterization of the exposed areas was conducted by electron backscatter diffraction (EBSD) and atomic force microscopy (AFM). First results indicate that the strain created by the FIB irradiation leads to a local transformation of beta gallium oxide to another polymorph.

HL 41.3 Thu 15:30 POT 81

Comparative Study of Temperature-dependent Bandgap Transitions in Ga2O3 Polymorphs — •Benjamin Moritz Janzen[1], Marcella Naomi Marggraf[1], Moritz Meissner[1], Nils Bernhardt[1], Conrad Valentin Hartung[1], Nima Hajizadeh[1], Felix Nippert[1], and Markus Raphael Wagner[1,2] — [1]Technische Universität Berlin, Institute of Solid State Physics, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany

We employ a combined experimental-theoretical study to investigate the electronic bandgap transitions in Ga2O3 polymorphs as a function of the sample temperature. For this purpose, we apply temperature-dependent UV photoluminescence excitation (PLE) spectroscopy for the β-, κ-, α- and γ-polymorphs in the temperature range between 5 and 300 K and compare the obtained bandgap values with room temperature measurements of the dielectric function as determined by spectroscopic ellipsometry. The obtained temperature dependencies are discussed in conjunction with DFT calculations regarding the effects of electron-phonon coupling.

HL 41.4 Thu 15:45 POT 81

Anisotropic IR active phonon modes and fundamental direct band-to-band transitions in α-$(Al_xGa_{1-x})_2O_3$ alloys grown by MOCVD — •Elias Kluth[1], A F M Anhar Uddin Bhuiyan[2], Lingyu Meng[2], Hongping Zhao[2], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, USA

The corundum-like Ga_2O_3 polymorph α-Ga_2O_3 is of high research interest as it allows bandgap-engineering by alloying e.g. with α-Al_2O_3, α-In_2O_3, α-Ti_2O_3 and similar materials. Since the corundum-like crystal structure is anisotropic, a direction dependent investigation of the material properties is crucial. m-plane α-$(Al_xGa_{1-x})_2O_3$ thin film samples up to x=0.76, grown on m-plane sapphire substrate by MOCVD have been investigated by infrared (IR) and visible-ultraviolet (UV) spectroscopic ellipsometry. IR ellipsometry yields the anisotropic IR active phonons and their shift to higher wavenumbers with increasing x. Furthermore, with UV ellipsometry, we find the anisotropic dielectric functions up to 6.6eV and the shift of the fundamental direct band-to-band transitions with increasing x. We report an anisotropic bowing parameter for α-$(Al_xGa_{1-x})_2O_3$ of b_{ord}=2.7eV and b_{extra}=2.5eV.

15 min. break

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Adsorption enhanced photocatalytic degradation of Rhodamine B using GdxBi1-xFeO3@SBA-15 (x= 0, 0.05, 0.10, 0.15) nanocomposites under visible light irradiation — •Thomas Cadenbach[1] and Maria Jose Benitez[2] — [1]Universidad San Francisco de Quito, Quito, Ecuador — [2]Escuela Politecnica Nacional, Quito, Ecuador

In the present work show that very high removal efficiency of a variety of organic pollutants by GdxBi1-xFeO3@SBA-15 nanocomposites (x = 0, 0.05. 0.10, 0.15) under visible light irradiation. Specifically, we study the photocatalytic degradation of dyes using the above nanocomposite materials, with pore volume loadings of 5-25%. We compare the obtained catalytic results for the nanocomposite materials to monodisperse BiFeO3 nanoparticles with a particle diameter of 5.5 nm. We find that the best removal performance is achieved by a 10 vol% Gd0.05Bi0.95FeO3@SBA-15 sample, shown by a complete dye degradation in approximately 3h using extremely low concentrations of the actural active photocatalyst. The superior efficiencies of the nanocomposites, which outperformed their parent compounds, i.e. GdxBi1-xFeO3 nanoparticles as well as unfilled SBA-15, are attributable to a synergistic adsorption enhanced photocatalytic degradation process. The possible mechanism in the photodegradation process was investigated and discussed on the basis of trapping experiments.

HL 41.6 Thu 16:30 POT 81

Electrical and thermal transport properties of $ZnGa_2O_4$ — Johannes Boy[1], Rüdiger Mitdank[1], Zbigniew Galazka[2], and •Saskia Fischer[1] — [1]Novel Materials Group, Humboldt-Univ. zu Berlin, Germany — [2]Leibniz-Institute of Crystal Growth, Berlin, Germany

The first full experimental determination of the low-temperature electrical, thermo-electrical [1] and thermal properties [2] of novel highly pure single crystalline $ZnGa_2O_4$ is reported. The temperature-dependences of the charge carrier density, mobility, and Seebeck coefficient including phonon drag are discussed between 10 K and 310 K. The thermal conductivity and diffusivity were determined by the so-called 2ω-method. At room temperature the electrical conductivity is 286 S/cm, the mobility 55 cm^2/Vs, the Seebeck coefficient 125$\mu V/K$ and the thermal conductivity is 22.9 W/mK. For temperatures above 100 K the phonon transport is limited by phonon Umklapp scattering. At lower temperatures boundary scattering at lattice defects limits the thermal conductivity to 95 W/mK. Therefore, if the cause of boundary scattering is reduced or eliminated, the thermal conductivity of $ZnGa_2O_4$ may be increased at low temperatures.

[1] J. Boy, *et al.*, AIP Advances 10, 055005 (2020) [2] J. Boy, *et al.*, Materials Research Express 9, 065902 (2022).

HL 41.7 Thu 16:45 POT 81

Temperature- and Polarisation- Dependant Photoluminescence Excitation Spectroscopy of $\beta - Ga_2O_3$. — •Moritz Meissner[1], Nils Bernhard[1], Felix Nippert[1], Benjamin M. Janzen[1], Conrad V. Hartung[1], Zbigniew Galazka[2], and Markus R. Wagner[1,3] — [1]Technische Universität Berlin, Institute of Solid State Physics, Berlin, Germany — [2]Leibniz-Initut für Kristallzüchtung, Berlin, Germany — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The anisotropic, ultra-wide bandgap semiconductor $\beta - Ga_2O_3$ represents a promising candidate for applications in high power electronics. The high anisotropy of the monoclinic crystal structure and the formation of self-trapped excitons has made a precise determination of the bandgap parameters a challenging endeavor. In this work, we apply polarization- and temperature-dependent photoluminescence excitation spectroscopy (PLE) measurements to study the anisotropy of the optical bandgap transitions. The temperature dependence of the PLE spectra between 5K and 300K provides information on the strength of the electron-phonon coupling and zero temperature bandgap energies along the principal axes of the material. The measurements were performed on the three crystal planes (100), (010) and (001) prepared and polished from the same single bulk crystal grown by the Czochralski method. Our results are discussed in comparison with absorption, transmission, and reflectance spectroscopy data in the literature.