β-Ga_2O_3 fundamental properties and their anisotropy

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To date, the fundamental material properties of Ga_2O_3 with its five different crystal modifications are not well experimentally characterized and tabulated yet. For all electrical purposes the relevant material parameters which need to be well known range from electrical properties such as the electrical conductivity based on the charge carrier density and mobility. Applications in high-power electronics furthermore require the consideration of the thermal conductivity and diffusivity as well as the thermal expansion coefficients. For all low-noise applications, any non-equilibrium leading to temperature differences across electrical contacts invokes thermovoltages. For their consideration in a device design the knowledge of the Seebeck coefficients are required. Finally, for any optical applications of the transparent Ga_2O_3 crystals or any high-frequency or gating application the knowledge of the dielectric constant is of particular interest. Interestingly, because of its monoclinic crystal structure, crystal anisotropy may play an important role in the material parameters and must be taken into account by the experimental measurement setup.

In the present funding period the project collaborations with the GraFOX research network have started intense work to attain reliable experimental values on β-Ga_2O_3 bulk single crystals, epitaxial layers and polycrystalline film. All samples were provided by the growth groups of PIs Günther Wagner and Zbigniew Galazka. Of particular interest was the investigation of

- anisotropy of the material parameters due to the intrinsic monoclinic crystal structure,
- influence of extrinsic growth defects such as twin boundaries or grain boundaries,
- doping, and
- for thin films the effect of surface and boundary effects.

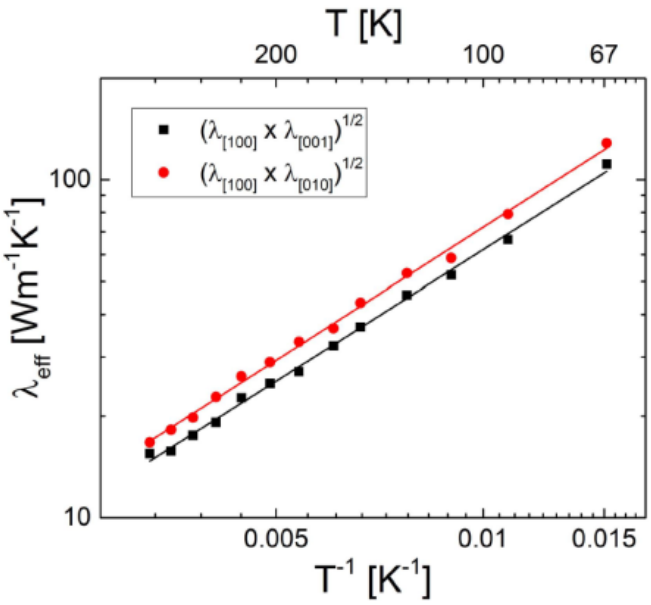
Within the GraFOx network we have

- identified the anisotropy of thermal conductivity and diffusivity of doped bulk crystals [1],
- ruled out any significant inherent anisotropy in the electrical conductivity [2],
- published the first values for Seebeck coefficients [3],
- measured the thermal expansion [4],
- and determined the anisotropy of the dielectric constant [5].

This required the implementation of novel measurement techniques, exchange of samples and discussion of the results from different experimental setups. All first authors of the publications are young researchers of the GraFOX projects.

Anisotropy of thermal conductivity and diffusivity bulk crystals [1]

In the project investigating thermal transport properties (PI Saskia Fischer) the temperature-dependent thermal conductivity λ and diffusivity D of a Mg-doped insulating β-Ga_2O_3 single crystal were determined along the [100], [010] and [001] directions. The so-called "2ω-method" was implemented by fabricating micrometer scale metal line heaters and thermometers directly on the crystal. The advantage of this method is that the anisotropy of λ can be obtained (simultaneously) from the same crystal. We detected a temperature-independent anisotropy factor of the thermal diffusivity and conductivity and find that the temperature dependence is in accord with phonon–phonon-Umklapp-scattering from 300 K down to 150 K. Below 150 K point-defect-scattering lowers the estimated phonon–phonon-Umklapp-scattering values. The room temperature values for the thermal conductivity in the main crystal axes are determined to 11 +/- 1 Wm^{-1} K^{-1} for [100], 29 +/- 2 Wm^{-1} K^{-1} for [010] and 21 +/- 2 Wm^{-1} K^{-1} for [001].



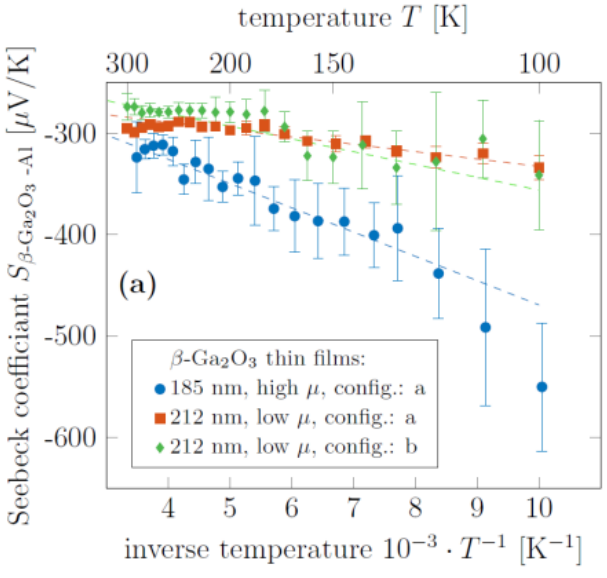
Electrical conductivity [2]

In the projects for electrical measurements on test devices (PIs W. Ted Masselink, Fariba Hatami together with PI Oliver Bierwagen) the electrical conductivity tensor of β-Ga_2O_3 was analyzed by van der Pauw measurements on differently oriented wafers in order to determine the inherent anisotropy, off-diagonal element, and the impact of grain boundaries. Despite the structural anisotropy a nearly isotropic conductivity was found by the determination of the 3-dimensional electrical conductivity tensor $\boldsymbol{\sigma}$. Analysis of the temperature dependence of the anisotropy and mobility of differently doped samples suggest this nearly isotropic behavior to apply for phonon-scattering as well as ionized-impurity scattering. We demonstrate that significantly higher anisotropies can be caused by extended structural defects in the form of low-angle grain boundaries for which we determine energy barriers of multiple 10 meV. Therefore we suggest to determine the conductivity anisotropy via the van der Pauw method as a quality control parameter to indicate growth-induced extended crystal defects.

$$\frac{\tilde{\sigma}^{a^*bc}}{\sigma_{bb}}(T = 300\ \mathrm{K}) = \begin{pmatrix} 1.01 \pm 0.04 & 0 & 0.05 \pm 0.03 \\ 0 & 1 & 0 \\ 0.05 \pm 0.03 & 0 & 0.96 \pm 0.01 \end{pmatrix}$$

Seebeck coefficient [3]

In the project investigating thermoelectrical transport (PI Saskia Fischer) the temperature dependence of the Seebeck coeffcient of epitaxial ß-Ga2O3 thin films was measured relative to aluminum. A specific micro-measurement platform with metallic line heaters and thermometers was implemented by laser-pattern lithography, sputter deposition and lift-of processing. For room temperature we find a relative Seebeck



coefficient of 300 +/- 20 µV/K. At high temperatures above 240 K, the scattering is determined by electron-phonon-interaction. At lower bath temperatures between 100 K and 300 K, an increase in the magnitude of the Seebeck coefficient is explained in the framework of Strattons formula. This leads to a room temperature Peltier coefficient of about 0.1 V. The dependency of the Seebeck coefficent on the dominant scattering mechanism gives the possibility of Seebeck coefficient engineering by growing β-Ga_2O_3 thin films with, for example, an increased concentration of neutral impurities or ionized impurities.

Thermal expansion [4]

The anisotropic coefficient of the thermal expansion $\boldsymbol{\alpha}$ for single-crystalline monoclinic β-Ga_2O_3 has been precisely measured by synchrotron-based high-resolution x-ray diffraction (PI Hanke) in the temperature range from 298 K to 1200 K. We derived values along the three main crystallographic directions, based on spacings for (600), (020) and (-204) lattice planes. α_a changes non-linearly between 0.10 x 10^{-6} K^{-1} and 2.78 x 10^{-6} K^{-1} in the temperature range of 298 K to 1200 K, while the values of α_b and α_c along the further two directions are nearly double. Within the Einstein model, we have numerically modeled the functional dependencies applying a single phonon mode.

Anisotropy of dielectric constant [5]

In the project for investigations of the (photo-)electrical transport in group-III sesquioxides (PI Klaus Irmscher) the static dielectric constant of β-Ga_2O_3 was measured using plate capacitor structures. The plate capacitors are made on the (100), (010) and (001) planes of pieces from a semi-insulating, Mg doped single crystal. The advantage of the plate capacitor method is that it determines ε_r directly. Our findings are: According to the monoclinic lattice of β-Ga_2O_3 the relative dielectric constant ε_r shows anisotropic values of 10.2 ± 0.2 (100), 10.87 ± 0.08 (010) and 12.4 ± 0.4 (001) at room temperature. ε_r is independent of the frequency in the range from 20 kHz to 1 MHz and there is only a weak dependence of ε_r on the temperature between 15 K and 500 K.

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GraFox publications are highlighted by an "*".