Phonon Mean Free Path - Thermal Conductivity Relation of Beta Form Gallium Oxide

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Beta-gallium oxide (β-Ga_2O_3) is an ultra-wide bandgap semiconductor material that has gained significant attention in recent years. With its wide bandgap over 4.5 eV it is found highly promising for high power and optoelectronic applications. Other uses include dielectric coatings for solar cells, deep-ultraviolet transistors, light-emitting diodes, and lasers [1]. The pressing issue of local heat build-up and narrowing thermal pathways in such high-performance miniature devices is a significant challenge and demands innovative solutions. This can be done by investigating the properties of dominant microscopic energy carriers in materials, in this case lattice vibrations (i.e., phonons). Such properties can help to understand the thermal behaviour of materials at the nanoscale. One of the critical properties that characterize this behaviour is the phonon mean free path (MFP). With its distinctive monoclinic lattice structure, β-Ga_2O_3 exhibits three-dimensional anisotropy in its thermal conductivity [2]. Therefore, additional problems in design and optimization of high-performance electronic devices made from this material are expected. The significantly lower conductivity (16-27 W/m.K at room temperature) compared to other wide-bandgap semiconductor materials like SiC and GaN [3] only complicates these problems. In this study, the phonon MFP and thermal conductivity relationships for (β-Ga_2O_3) at different lattice temperatures were theoretically derived through ab-initio simulations and phonon interaction computations, using up to third-order force constants. Our results reveal that the isotopic disorder of gallium atoms is the main factor that affects the phonon mean free path, while anharmonic phonon-phonon interactions cause a plateau-like behaviour in thermal conductivity at low temperatures.

References

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[3] Guo Z, Verma A, Wu X, Sun F, Hickman A, Masui T, Kuramata A, Higashiwaki M, Jena D, Luo T. Applied Physics Letters. Anisotropic thermal conductivity in single crystal β-gallium oxide. 2015 Mar 16;106(11):111909.

Figures

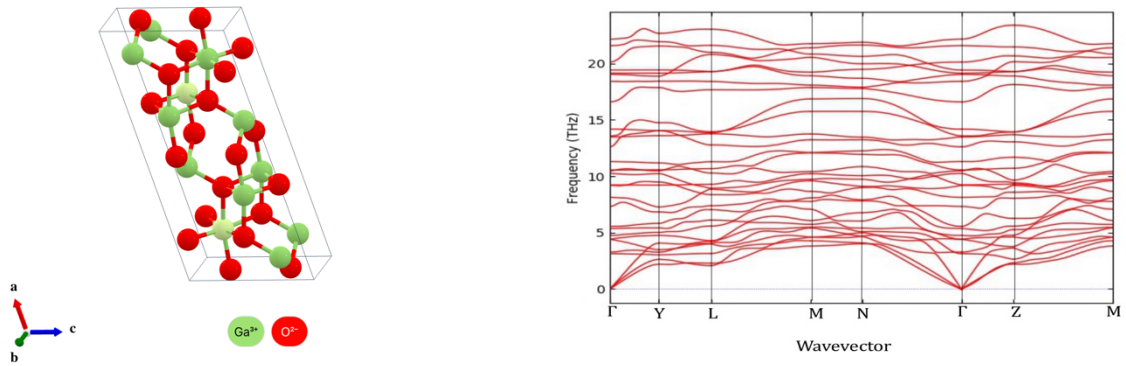

Figure 1. (Left) The unit cell and (Right) Phonon dispersion of β-Ga_2O_3