Anisotropic Phonon Scattering at Grain Boundaries in Nanocrystalline β-Ga_2O_3 Under High-Flux Neutron Irradiation: A Defect-Mediated Thermal Transport Analysis

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Abstract. This study investigates anisotropic phonon scattering mechanisms at grain boundaries in nanocrystalline β-phase gallium oxide (β-Ga_2O_3) subjected to high-flux neutron irradiation at fluences ranging from 10^{16} to 10^{19} n/cm². Using time-domain thermoreflectance (TDTR) spectroscopy combined with molecular dynamics (MD) simulations employing embedded-atom method potentials, we quantify defect-mediated suppression of thermal conductivity along the [010] and [001] crystallographic axes. Irradiation-induced Frenkel pair accumulation and interstitial oxygen clustering were identified as dominant scattering centers, reducing anisotropic thermal conductivity by up to 67% at peak fluence. Phonon lifetime analysis via Green–Kubo autocorrelation functions reveals preferential umklapp scattering along monoclinic off-axis directions. These findings provide a quantitative framework for predicting thermal degradation in β-Ga_2O_3-based power electronics and neutron-environment semiconductor devices.

Keywords: β-Ga_2O_3 thermal transport, anisotropic phonon scattering, neutron irradiation-induced defects, nanocrystalline grain boundary resistance, time-domain thermoreflectance, Frenkel pair accumulation, umklapp scattering anisotropy, wide-bandgap semiconductor degradation, molecular dynamics phonon lifetime

Introduction

The thermal management of wide-bandgap semiconductors operating in extreme radiation environments represents one of the most pressing challenges in contemporary condensed matter physics and materials science, with direct implications for next-generation nuclear power systems, space-borne electronics, and high-power device engineering as of 2024–2026. Among ultra-wide-bandgap candidates, β-phase gallium oxide (β-Ga_2O_3) has attracted intense scrutiny owing to its exceptionally high Baliga figure of merit (~3,444 relative to silicon), theoretical breakdown electric field exceeding 8 MV/cm, and inherent monoclinic crystal symmetry that produces pronounced intrinsic anisotropy in phononic transport. However, the deployment of β-Ga_2O_3 in neutron-rich environments—such as those encountered in fission reactor instrumentation, tokamak diagnostics, and satellite power conditioning circuits—introduces a secondary and poorly understood complication: the systematic generation of radiation-induced point defects, dislocation loops, and oxygen interstitial clusters that act as parasitic phonon scattering centers, severely attenuating the already anisotropic thermal conductivity tensor of the host lattice. Previous investigations into radiation effects in β-Ga_2O_3 have largely focused on carrier displacement damage thresholds, Hall mobility degradation, and Schottky barrier modification under proton or gamma irradiation. Comparatively little attention has been directed toward the grain-boundary-mediated phonon transport regime under neutron bombardment, particularly within polycrystalline and nanocrystalline morphologies where interfacial Kapitza resistance and boundary dislocation density play non-negligible roles in the effective medium thermal conductivity. The monoclinic unit cell of β-Ga_2O_3, belonging to space group C2/m, presents inequivalent Ga(I) tetrahedral and Ga(II) octahedral sublattice sites, both of which exhibit distinct displacement energies and defect formation enthalpies under ballistic recoil cascades, further complicating predictive defect–phonon interaction models. This paper addresses the foregoing gap by presenting a combined experimental and computational analysis of anisotropic phonon scattering at grain boundaries in nanocrystalline β-Ga_2O_3 samples irradiated at a research fission reactor to controlled neutron fluences. The study is structured as follows: Section 2 details the sample fabrication, neutron irradiation protocol, and TDTR experimental configuration; Section 3 presents the MD simulation methodology, including interatomic potential benchmarking and Green–Kubo thermal conductivity extraction procedures; Section 4 reports measured and simulated anisotropic thermal conductivity as a function of fluence and grain size; Section 5 discusses defect speciation via positron annihilation spectroscopy and its correlation with phonon lifetime suppression; and Section 6 synthesizes the results into a predictive defect-accumulation thermal degradation model applicable to real device geometries.

References

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