

Theory of the lattice thermal conductivity in bulk and films of GaN

A. AlShaikhi,¹ Saswati Barman,² and G. P. Srivastava³

¹*Physics Department, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia*

²*Department of Material Sciences, S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Saltlake, Kolkata 700098, India*

³*School of Physics, University of Exeter, Stocker Road, Exeter EX4 4QL, United Kingdom*

(Received 13 March 2010; revised manuscript received 2 May 2010; published 27 May 2010)

We report on a systematic theoretical investigation of the lattice thermal conductivity of several GaN samples (bulk and films) over a wide range of temperature, by applying Callaway's relaxation-time theory in its full form and Srivastava's scheme for anharmonic three-phonon scattering processes. The role of the usually neglected three-phonon normal-drift term has been quantified. We have attempted to quantify the role of phonon scattering by various defects and imperfections, present in the film samples, in controlling the temperature dependence of thermal conductivity. We find that except for the purest sample, the phonon-impurity scattering plays a significant role in controlling the thermal conductivity of GaN not only around the thermal-conductivity peak region but also over a very large range of temperature. It can also be predicted from our numerical study, and with available experimental results, that the highest possible thermal conductivity of bulk GaN can only be realized when point impurities such as oxygen and silicon are in small concentration ($\approx 10^{16}$ cm⁻³ or less) and other defects are either absent (from experimental study) or present in very small concentration (our numerical study). The highest value of the room-temperature thermal conductivity is achieved for samples grown by the high-temperature and high-pressure growth technique.

DOI: [10.1103/PhysRevB.81.195320](https://doi.org/10.1103/PhysRevB.81.195320)

PACS number(s): 65.40.-b, 63.20.kp

I. INTRODUCTION

Due to the wide range of potential applications, gallium nitride (GaN) has been receiving an extensive and growing research attention. GaN-based proposed technologies include applications in high-power electronic devices, light-emitting diodes, laser diodes, ultrapower switches, and microwave-power sources. Reliable performance of such devices depend on the heat dissipation in the active regions. Therefore, the thermal conductivity of GaN plays a key role in controlling the performance of GaN-based devices. GaN is one of the 12 "high thermal conductivity" nonmetallic materials.¹ This advantage allows GaN to be an excellent candidate for device applications. Since heat conduction in semiconductors is primarily due to phonons, understanding various phonon-scattering processes in limiting the thermal conductivity of GaN is extremely important for device design and improvement of device performance. The lattice thermal conductivity of most of the semiconducting materials such as diamond, Si, and Ge is controlled by the point-impurity defect scattering around the thermal-conductivity peak region and by the anharmonic three-phonon scattering at room temperature and beyond that. In contrast, it has been found that the temperature dependence of the thermal conductivity of bulk GaN and GaN films deviates from that in most of the semiconducting materials. Due to different growth techniques used, H, Si, and Ga vacancies, unintentionally doped impurities such as oxygen, oxygen-related defects, and various other defects form sources of phonon scattering, severely limiting the thermal conductivity of GaN over a wide range of temperature. GaN films grown on foreign substrates contain structural imperfections such as dislocations due to the presence of the strain field arising from the lattice mismatch between the substrate and the film.

Such imperfections also scatter the heat-carrying phonons and thereby limit the phonon thermal conduction. These extra scattering processes may become one of the main causes of different temperature dependence of the thermal conductivity of GaN as compared to other materials.

Sichel and Pankove² made the first measurements of the thermal conductivity of 400- μ m-thick GaN film grown by hydride vapor-phase epitaxy (HVPE) in the temperature range 25–360 K and obtained the room-temperature thermal-conductivity value ~ 130 W m⁻¹ K⁻¹ along the *c* axis. Asnin *et al.*³ measured the room-temperature thermal-conductivity value of a lateral epitaxial overgrown (LEO) GaN film using the scanning thermal microscopy technique and reported the thermal-conductivity values to be in the range 170–180 W m⁻¹ K⁻¹. Using the third harmonic electrical (3ω) technique, Luo *et al.*⁴ found the room-temperature thermal conductivity of ~ 155 W m⁻¹ K⁻¹ for LEO GaN of 5 μ m thickness, a value significantly higher than previously reported for bulk GaN. This is believed to be due to substantially lower amount of dislocation density in the LEO film (less than 5×10^6 cm⁻²).⁴ In comparison, the HVPE-grown GaN films usually have higher dislocation density on the order of 10^{10} cm⁻². In a following work, Luo *et al.*⁵ presented results for the thermal conductivity of LEO GaN over the temperature range 60–300 K. Kamano *et al.*⁶ measured the thermal conductivity of bulk GaN in the temperature range 110–370 K by photothermal divergence method and predicted that the phonon-defect scattering may play a crucial role near the room temperature. In 2002, Slack *et al.*⁷ employed the steady-state heat-flow technique to measure the thermal conductivity of a 200- μ m-thick and 3000- μ m-wide GaN sample prepared by the HVPE technique and reported the room-temperature value as 227 W m⁻¹ K⁻¹. Jeżowski *et al.*^{8–10} have measured the