TEMPERATURE DEPENDENCE OF THE THERMAL CONDUCTIVITY OF WURTZITE ALUMINUM NITRIDE, GALLIUM NITRIDE AND ALUMINUM-GALLIUM NITRIDE

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I. INTRODUCTION

Over the last decades, much attention has been focused on III-nitride semiconductors aluminum nitride (AlN), gallium nitride (GaN) and aluminum-gallium nitride (AlGaN) as promising materials for the application in high-power radio-frequency electronic and optoelectronic devices. Although the structural, electronic and optical properties have been extensively studied, relatively little work, both analytical and experimental, has

to date been reported on their thermal conductivity (κ). Meanwhile, this thermoelectric parameter a measure of the ability to conduct heat is important from both fundamental and applied aspects [1].

In this paper, we make a thorough analysis of the structural and phonon properties of wurtzite AlN, GaN and AlGaN in the framework of the *ab initio* (or "first-principles") formalism [2] to determine the thermal conductivity at various temperatures (T).

II. CALCULATION PROCEDURE

The first-principles method combines an exact iterative solution of the phonon Boltzmann transport equation in the single-mode relaxation time approximation with accurate computations of the second-order (harmonic) and third-order (anharmonic) interatomic force constants. We perform the first-principles calculations using a plane-wave basis set within the framework of the density-functional theory as implemented in the Vienna Ab initio Simulation Package [3]. The Perdew-Burke-Ernzerhof parameterization is employed for the exchange-correlation functional [4]. Projector-augmented wave potentials are used for Al, Ga and N atoms and the plane-wave cutoff energy is set to 520 eV. For the determination of the third- and second-order force constants, reciprocal spaces of the α-quartz supercells are sampled by the 3×3×3 mesh and at Γ point only, respectively. Non-self-consistent calculations are made along the lines between the high-symmetry points L-Γ-X and M-K-Γ-A of the first Brillouin zone.

III. RESULTS

Figure 1 shows the temperature dependence of the thermal conductivity of defect-free wurtzite AlN and GaN. The thermal conductivity at 300 K of AlN (GaN) along the [100] and [001] crystal directions is calculated to be 3.96 (2.59) and 4.62 (3.36) W/(cm·K), yielding an anisotropy factor of 1.17 (1.30). As the temperature grows to 700 K, the κ values of 1.37 (1.08) and 1.58 (1.36) W/(cm·K) are obtained, leading to an anisotropy factor of 1.15 (1.26) a slight decrease relative to the figures observed at very low temperatures. In a range from 300 to 700 K, the κ curves for AlN [100] and AlN [001] have slopes of -1.28 and -1.29. The thermal conductivity of GaN [100] and GaN [001] falls off as $T^{-1.03}$ and $T^{-1.07}$, respectively.

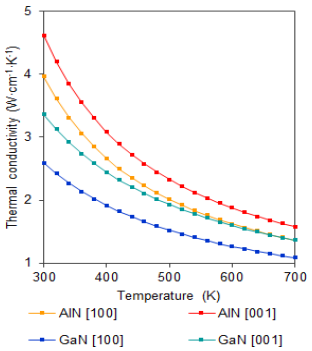

Figure 1. Thermal conductivity of wurtzite AlN and GaN as a function of temperature

In Figure 2, the dependence of the thermal conductivity of defect-free wurtzite $Al_xGa_{1-x}N$ on composition (x) at different temperatures is given. In semiconductor alloys fabricated from AlN and GaN, the resistive phonon-phonon scattering increases greatly resulting in κ values far lower than those of their end-point materials. At 300 K, $Al_{0.42}Ga_{0.58}N$ [100] and $Al_{0.48}Ga_{0.52}N$ [001] are characterized by the lowest thermal conductivity of 1.83 and 1.63 W/(cm·K), respectively. In a range from 300 to 700 K, the bowing parameter can be approximated by $3.649118 \cdot 10^{-3}T$ - 0.2210367 for $Al_xGa_{1-x}N$ [100] and by $6.390055 \cdot 10^{-3}T$ - 0.5105837 for $Al_xGa_{1-x}N$ [001].

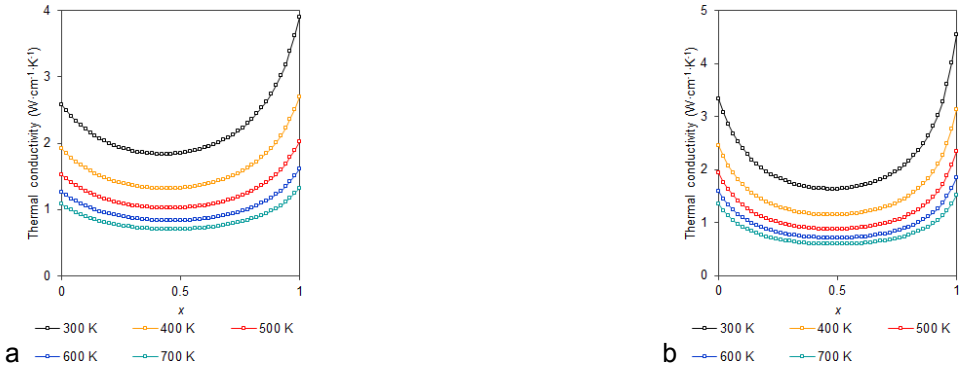

Figure 2. Thermal conductivity of wurtzite $Al_xGa_{1-x}N$ as a function of composition at various temperatures: a – [100]; b – [001]

IV. CONCLUSIONS

We have made a careful analysis of the structural and phonon properties of wurtzite AlN, GaN and AlGaN in the framework of the *ab initio* formalism to determine their thermal conductivity at various temperatures. The mathematical models for κ that account for crystal direction, composition and temperature were presented.

ACKNOWLEGMENTS

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