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Temperature Dependence of the Thermal Conductivity of Wurtzite Aluminum Nitride, Gallium Nitride and Aluminum-Gallium Nitride

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Introduction

- Over the last decades, a lot of 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 microwave electronic and optoelectronic devices[1,2]. The intense interest in these semiconductors arises from the following factors. First, the wide band gaps of AlN and GaN yield high breakdown voltages, which is valuable for high-power device operation. Second, the high saturation velocity of electrons in AlN and GaN enables high-frequency operation. Furthermore, the natural structure of AlN and GaN is wurtzite—a hexagonal crystal structure where electrical polarization effects play a major role[3]. At heterojunctions formed by III-nitrides, the polarization induces a very high electron concentration, providing a large current density.
- Although the structural, electronic and optical properties have been extensively studied, relatively little work, both analytical and experimental, has to date been reported on the thermal conductivity (κ) of AlN, GaN and, especially, AlGaN. Meanwhile, this thermoelectric parameter—a measure of the ability to conduct heat—is significant from both fundamental and applied aspects.
- In this work, we made 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[4] to determine their thermal conductivity at various temperatures (*T*).

Computation 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. The second-order interatomic force constants are required for the calculation of the phonon dispersion relation, while the third-order constants are necessary for the calculation of the three-phonon scattering rates.
- The first-principles electronic structure calculations were performed using a plane-wave basis set in the framework of the density-functional theory as implemented in the *Vienna Ab initio Simulation Package*[5]. The first-principles phonon calculations necessary for the determination of the thermal properties were carried out by the open-source *Phonopy* package[6]. The thermal conductivity calculations were carried out by the open-source *Phono3py* package[7].

1 VASP Electronic structure calculations from first principles

2 Phonopy Phonon calculations from first principles

3 Phono3py Thermal conductivity calculations

Fig. 1. Thermal conductivity computation procedure

- The advantage of the method is that no adjustable parameters are invoked as the interatomic force constants are the only input parameters required for the exact solution.
- The thermal conductivity obtained by solving the phonon Boltzmann transport equation is expressed as below.

$$\kappa = \frac{1}{\kappa_B T^2 N V} \sum_{\zeta} (\hbar\omega)^2 \overline{n}_{\zeta} \left(\overline{n}_{\zeta} + 1\right) v_{\alpha\zeta} d_{\beta\zeta} \quad (1)$$

- κ_B Boltzmann constant
- N number of discretizing $\vec{q}$ points in the Brillouin zone
- V volume of the primitive unit cell
- ζ phonon mode $(\vec{q}, j)$
- j phonon polarization type
- $\hbar$ reduced Planck constant
- ω phonon frequency
- $\bar{n}$ phonon group equilibrium population
- v phonon group velocity
- d mean free displacement
- α, β Cartesian directions

Results

- Since the thermal conductivity values calculated from first principles come in tabulated form, a power function that has the best fit to the respective values in a temperature range from 300 to 700 K was constructed for each of the materials.

AlN

$$\kappa^{\mathrm{AlN}[100]} = 3.89\left(\frac{T}{300}\right)^{-1.28} \quad (2)$$

$$\kappa^{\mathrm{AlN}[001]} = 4.53\left(\frac{T}{300}\right)^{-1.29} \quad (3)$$

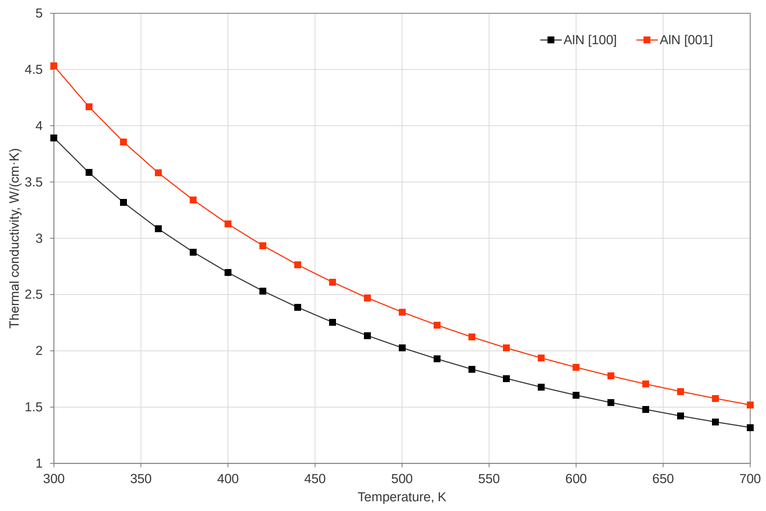

Fig. 2. Temperature dependence of the thermal conductivity of AlN

GaN

$$\kappa^{\mathrm{GaN}[100]} = 2.58\left(\frac{T}{300}\right)^{-1.03} \quad (4)$$

$$\kappa^{\mathrm{GaN}[001]} = 3.34\left(\frac{T}{300}\right)^{-1.07} \quad (5)$$

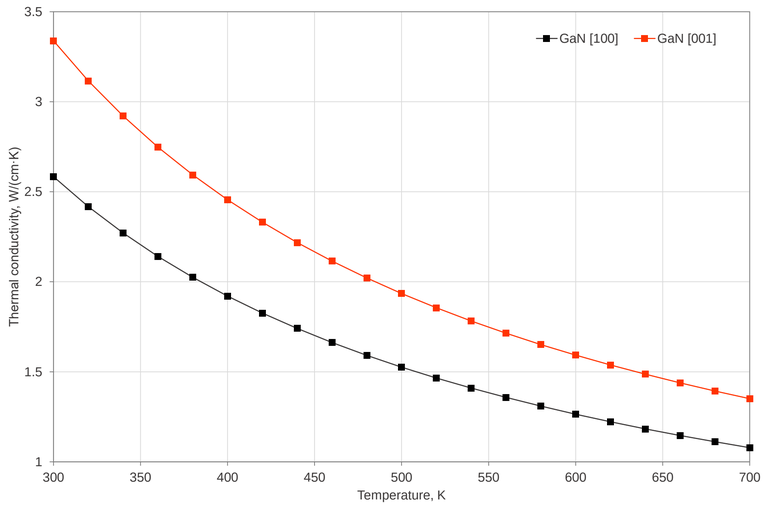

Fig. 3. Temperature dependence of the thermal conductivity of GaN

AlGaN

$$\kappa^{\mathrm{AlGaN}[100]} = \left(\frac{x}{\kappa^{\mathrm{AlN}[100]}} + \frac{1-x}{\kappa^{\mathrm{GaN}[100]}} + C^{\mathrm{AlGaN}[100]} x(1-x)\right)^{-1} \quad (6)$$

$$\kappa^{\mathrm{AlGaN}[001]} = \left(\frac{x}{\kappa^{\mathrm{AlN}[001]}} + \frac{1-x}{\kappa^{\mathrm{GaN}[001]}} + C^{\mathrm{AlGaN}[001]} x(1-x)\right)^{-1} \quad (7)$$

$$C^{\mathrm{AlGaN}[100]} = 3.649118\times10^{-3}T - 0.221037 \quad (8)$$

$$C^{\mathrm{AlGaN}[001]} = 6.390055\times10^{-3}T - 0.510584 \quad (9)$$

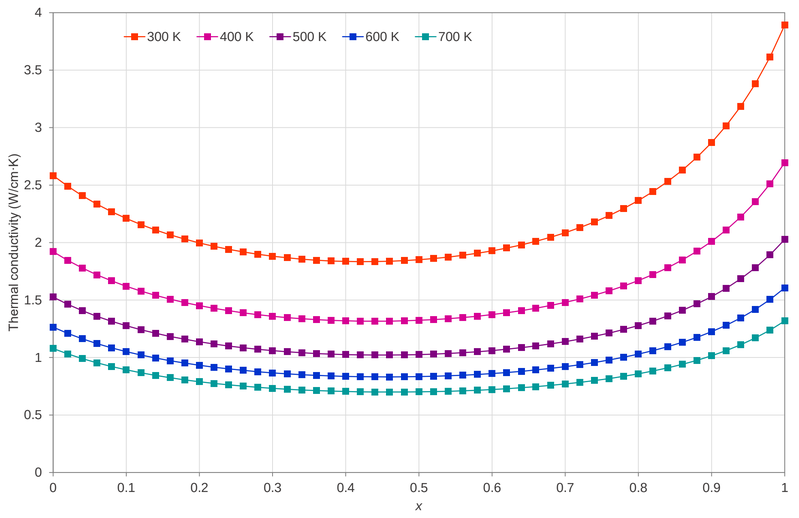

Fig. 4. Thermal conductivity of $Al_xGa_{1-x}N$ [100] as a function of composition (x) at various temperatures

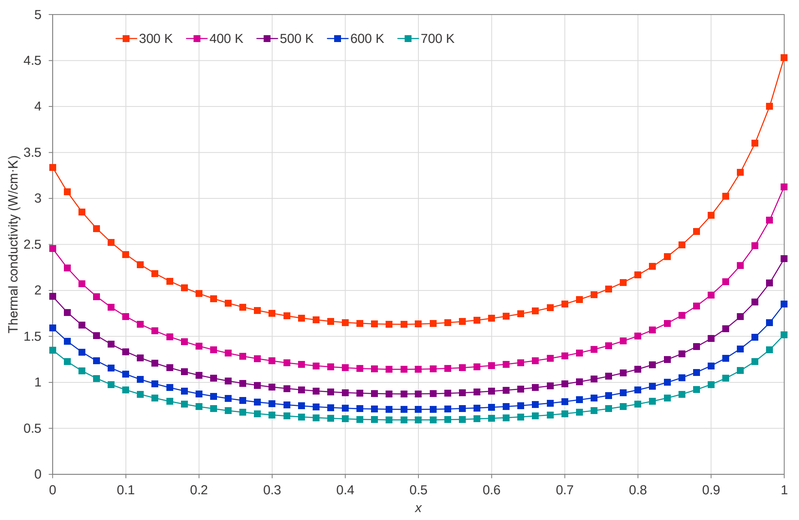

Fig. 5. Thermal conductivity of $Al_xGa_{1-x}N$ [001] as a function of composition at various temperatures

Conclusions

- A careful analysis of the structural and phonon properties of wurtzite AlN, GaN and AlGaN was made 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.
- 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.

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