Thermal transport properties of GaN with biaxial strain and electron-phonon coupling Image: Strain and Electron-phonon coupling

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ABSTRACT

Strain inevitably exists in practical GaN-based devices due to the mismatch of lattice structure and thermal expansion brought by heteroepitaxial growth and band engineering, and it significantly influences the thermal properties of GaN. In this work, thermal transport properties of GaN considering the effects from biaxial strain and electron-phonon coupling (EPC) are investigated using the first principles calculation and phonon Boltzmann transport equation. The thermal conductivity of free GaN is 263 and 257 W/mK for in-plane and cross-plane directions, respectively, which are consistent better with the experimental values in the literature than previous theoretical reports and show a nearly negligible anisotropy. Under the strain state, thermal conductivity changes remarkably. In detail, under +5% tensile strain state, average thermal conductivity at room temperature decreases by 63%, while it increases by 53% under the -5% compressive strain, which is mostly attributed to the changes in phonon relaxation time. Besides, the anisotropy of thermal conductivity changes under different strain values, which may result from the weakening effect from strain induced piezoelectric polarization. EPC is also calculated from the first principles method, and it is found to decrease the lattice thermal conductivity significantly. Specifically, the decrease shows significant dependence on the strain state, which is due to the relative changes between phonon-phonon and electron-phonon scattering rates. Under a compressive strain state, the decreases of lattice thermal conductivity are 19% and 23% for in-plane and cross-plane conditions, respectively, comparable with those under a free state. However, the decreases are small under the tensile strain state, because of the decreased electron-phonon scattering rates and increased phonon anharmonicity.

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I. INTRODUCTION

Gallium nitride (GaN), a representative wide bandgap semiconductor, has attracted much attention in the past few decades as a candidate material for advanced power electronic devices.^{1,2} Due to its wide bandgap (up to 3.4 eV) and high electron saturation velocity, GaN can suffer from higher breakdown voltage and higher temperature compared with traditional semiconductors and is suitable for applications in high-frequency, high-efficiency, and highpower devices.^{3,4} In the device level, a GaN-based IC, e.g., high electron mobility transistors (HEMTs), performs very well in aspects of electron mobility and electron density.^{5–8} In spite of these advantages, GaN devices are also faced with challenges in the heat dissipation issue raised by high power and high integrity density. Since high temperature in a hot spot will cause serious damage on reliability and lifetime of devices,⁹ an understanding on the thermal process in GaN-based devices and accurate thermal modeling are highly desired.

Taking AlGaN/GaN HEMT as an example (Fig. 1), the thermal processes in the devices include heat generation near the gate and thermal transport from the top layer to the substrate. First, heat is generated at the top of the channel layer as Joule heating, where two-dimensional electron gas is formed. Then, heat spreads in both in-plane and cross-plane directions in the channel layer. Furthermore, heat will transport across the transition layer and finally dissipate to the substrate and outer heat sink. It can be known from the thermal process analyses that thermal spreading resistance across the GaN layer dominates thermal transport inside the HEMTs,¹⁰ where thermal conductivity and interfacial thermal



FIG. 1. Schematic of a simplified GaN-based HEMT structure.

conductance are basic properties for further thermal modeling and predictions.

In the last two decades, both experimental and calculation data of GaN thermal conductivity have been reported, as shown in Table I. For experimental data in the literature, they differ significantly among each other, ranging from 145 to 280 W/mK. This can

TABLE I. Experimental and calculated values of GaN thermal conductivity at room temperature.

Data cources	Maximum	Mathada
Data sources	values (w/mk)	Methods
Asnin et al. ¹¹	180	Scanning thermal microscope
Florescu <i>et al.</i> ¹²	210	
Jeżowski <i>et al.</i> ¹³	269	Axial stationary heat flow
Slack <i>et al</i> . ¹⁴	220	method
Jeżowski <i>et al.</i> ¹⁵	230	
Jagannadham <i>et al.</i> ¹⁶	280	3-Omega
Churiukova	280	
et al."		
Luo et al. ¹⁸	155	
Paskov <i>et al.</i> ¹⁹	243	
Rounds <i>et al.</i> ²⁰	224	
Mion <i>et al.</i> ²¹	230	
Kamano <i>et al.</i> ²²	145	TTR (Transient
		thermo-reflection)
Beechem	180	TDTR (Time-domain
<i>et al.</i> ²³		thermo-reflection)
Zheng <i>et al.</i> ²⁴	249	
Shibata et al. ²⁵	253	Laser flash
Lindsay <i>et al.</i> ²⁶	400	First principle-based phonon
Garg et al. ²⁷	390	Boltzmann transport equation
Yang et al. ²⁸	420	(BTĒ)
Yuan et al. ²⁹	330	

be attributed to the following reasons. The first one is that the quality of a GaN crystal varies in different experiments due to the different substrates used in heteroepitaxial growth. Secondly, thermal conductivity may depend on the thickness of thin GaN films.^{10,30,31} Finally, different measurement methods have been used in experiments, including 3-Omega, time-domain thermoreflection (TDTR), laser flash method, and so on, which may introduce a difference in final experimental results. The first principles calculation based phonon Boltzmann transport equation (BTE) is promising for providing reliable thermal conductivity results.³ However, thermal conductivity data of GaN from first principles calculations in the currently available literature show unsatisfied consistency yet. The highest thermal conductivity reported is up to 420 W/mK, much higher than the highest experimental value of 280 W/mK. Lindsay et al. ²⁶ reported that the thermal conductivity of GaN at room temperature can be as high as 400 W/mK and attributed the lower thermal conductivity in experiments to the isotope effects. Garg et al.27 investigated the spectral phonon properties and thermal conductivity and found that contribution to thermal conductivity from phonons of frequency 5-7 THz exceeds 60% where total thermal conductivity is 390 W/mK. Yang et al.²⁴ considered the contribution from electron-phonon coupling (EPC) in lattice thermal conductivity calculations and pointed out that EPC decreases thermal conductivity by about 30% where the original value is 420 W/mK. Yuan et al.²⁹ analyzed the effects of functionals in first principles calculations, and the calculated thermal conductivity is 330 W/mK. In fact, empirical settings or parameters are still needed in practical first principles calculations, such as kinetic energy cutoff in-plane wave expansions, supercell size in force constant calculations, and choice of functionals and pseudopotentials. Furthermore, how to determine the final lattice parameters remains unclear. Therefore, these empirical settings and parameters should be tested systematically and carefully.

The thermal conductivity of GaN is affected by many factors in real devices, including strain, dislocation, point defect, size, doping, etc.^{1,2,10} Generally, GaN is grown on a foreign substrate, i.e., heteroepitaxial growth, since it is still unavailable for the large-scale single crystal growth of GaN. Mismatches in the lattice structure and thermal expansion exist between GaN and these substrates,^{33–37} introducing a remarkable in-plane biaxial strain in the channel layer,^{33,38,39} and inducing high dislocation density in the GaN layer,⁴⁰⁻⁴⁴ which is now a burning problem for material scientists. To release the strain in a channel layer, the transition layer is usually inserted to decrease the mismatch (Fig. 1). However, the strain is still non-negligible in most conditions. Actually, in the perspective of property tuning, strain is also necessary in devices. Specific strain is required for designing electronic properties through band engineering. Also, strain can be applied as a positive method to control electron and photon properties, as well as phonon thermal properties, since these properties are sensitive to the strain state.⁴⁵ At present, band engineering with strain has been widely used for many materials including twodimensional and three-dimensional semiconductors.46-51 In devices with band engineering, lattice thermal conductivity will also be influenced with no doubts.

Investigations on strain effects and strain engineering on thermal conductivity of solids have been widely carried out during

the past few decades in materials such as metal and semiconductor nanostructures,^{52–55} Lennard-Jones systems,^{56,57} polymer,⁵⁸ bulk silicon,⁵⁶ typical semiconductors on substrates,⁵⁹ heterostructures,⁶ and low-dimensional materials.⁶¹⁻⁶⁵ In fact, strain can not only tune the absolute value of thermal conductivity but also the anisotropy of thermal conductivity and the dependence of thermal conductivity on temperature and system size.⁶⁶ In principle, strain can influence the thermal properties significantly by changing lattice constants, the structure phase, and symmetry of systems.⁵⁹ Generally, response of thermal conductivity to strain differs for different responses of phonon properties. As reported in Ref. 56, thermal conductivity of Lennard-Jones systems monotonously increases under compressive the strain state and decreases under the tensile strain state. While thermal conductivity of silicon keeps a constant under compressive strain state and decreases under tensile strain state, strain effects on the thermal conductivity of GaN based on first principles calculations are still lacking.

In intrinsic nonpolar covalent semiconductors, EPC can be ignored for phonon thermal transport. However, it is non-negligible for semiconductors with high doping density and polar semiconductors in which electron-polar-optical-phonon interaction is significant. Liao *et al.*⁶⁸ have performed calculations of thermal conductivity with EPC in heavily doped silicon of which the thermal conductivity greatly decreases with the increase of doping density. Yang *et al.* reported the importance of strong coupling between electrons and long-wavelength longitudinal optical phonons in calculating the thermal conductivity of GaN.²⁸ Since electronic properties are sensitive to strain as mentioned above, the EPC in polar materials is then expected to be affected by strain remarkably. Hence, strain effects on EPC and its role in lattice thermal conductivity should be included in the investigations of strain effects on lattice thermal conductivity.

In this work, the effects of in-plane biaxial strain on phonon properties and thermal conductivity of GaN are systematically investigated using the first principles calculation based phonon Boltzmann transport equation considering the contribution from EPC. It is found that the lattice thermal conductivity of GaN changes monotonously and significantly under strain states, namely, it decreases under the tensile strain state and increases under the compressive strain state. Besides, the decreases of lattice thermal conductivity brought by EPC are also analyzed, which is significantly dependent on the strain states.

II. METHODS

The density functional theory based first principles calculations in this work mainly includes two parts. One is the first principles calculations on phonon harmonic and anharmonic properties of wurtzite structure GaN. The other is the first principles calculations on EPC, which will be described in the next paragraph. The first part is performed with a Vienna *ab initio* Simulation Package (VASP)⁶⁹ using projective augmented wave (PAW) pseudopotential⁷⁰ and the generalized gradient approximation in the Perdew-Burke-Ernzerhof (PBE) form⁷¹ for the exchange-correlation functional. Following suggestions from the VASP manual, Ga_d pseudopotential is selected for gallium atoms, where the *d* orbit electrons are treated as valence orbital electrons. The necessity of this choice was pointed out by Fiorentini *et al.*⁷² for the energy resonance of Ga 3*d* states with N 2s states and was validated by Yuan et al.²⁹ The kinetic energy cutoff for plane wave basis 800 eV is employed in solving the Kohn-Sham equations in VASP. The Brillouin zone is sampled using converged $10 \times 10 \times 10$ Monkhorst-Pack k-mesh grids⁷ with a careful convergence test. In the structural optimization step, the atom positions and lattice constants are fully relaxed until the residual stress and the maximum forces acting on each atom are smaller than 10^{-2} kbar and 10^{-6} eV/Å, respectively. Phonon harmonic properties including phonon density of states (DOS) and phonon dispersion relations require the second order interatomic force constants (IFCs), while phonon anharmonic properties require the third order interatomic force constants. In this work, we take the former one by using the density functional perturbation theory (DFPT) method as implemented in VASP and the Phonopy package⁷⁴ with a $4 \times 4 \times 3$ supercell. Since VASP calculates force constants at the gamma point only with DFPT, a large supercell is still needed for accurate results. The Born effective charges and high-frequency dielectric constants are also calculated with DFPT for nonanalytical corrections in phonon dispersion calculations brought from polar effects.^{75,76} For the third order IFCs, a finite displacement supercell method (also called the frozen phonon method)⁷⁶ is used with a $5 \times 5 \times 3$ supercell, and the interaction cutoff is up to fifth-nearest neighbors based on a previous convergence test.²¹ By solving the eigenvalue equation of phonons and using the Fermi golden rule, phonon dispersion relation, group velocity, DOS, and relaxation time can be obtained. Then, lattice thermal conductivity can be calculated by solving the phonon Boltzmann transport equation with an iterative method,

$$\boldsymbol{\kappa}_{L}^{\alpha\beta} = \frac{1}{k_{B}T^{2}\Omega N} \sum_{\boldsymbol{q}\nu} f_{0}(f_{0}+1)(\hbar\omega_{\boldsymbol{q}\nu})^{2} \boldsymbol{\nu}_{\boldsymbol{q}\nu}^{\alpha} F_{\boldsymbol{q}\nu}^{\beta}, \qquad (1)$$

where f_0 is the Bose-Einstein distribution function, $\omega_{\mathbf{q}\nu}$ is the phonon angular frequency in wavevector **q** and polarization ν , and ν is the phonon group velocity. *F* is the product of phonon group velocity and converged relaxation time $v_{\mathbf{q}\nu}^{\beta}\tau_{\mathbf{q}\nu}^{0}$, in the dimension of distance, and can be simplified into $v_{\mathbf{q}\nu}^{\beta}\tau_{\mathbf{q}\nu}^{0}$ under relaxation time approximation (RTA) where τ^0 is the phonon relaxation time from the perturbation theory.

In polar crystals, EPC is promised to be remarkable as mentioned in Sec. I. Besides the typical coupling between electron and acoustic longitudinal phonons, which is usually modeled as acoustic deformation potential in the literature, another important part is coupling between electron and long-wavelength longitudinal polar optical phonons, which is called Fröhlich interaction, a typical characteristic in polar crystal. In this work, DFPT and Wannier interpolation methods are used to calculate EPC. In detail, electron and phonon wavevectors and dynamical matrix, and electron-phonon interaction matrix are firstly calculated in coarse mesh grids by the DFPT method as implemented in Quantum ESPRESSO⁷⁷ and then interpolated in fine mesh grids with the Electron-Phonon Wannier (EPW) package⁷⁸ using the Maximized Localized Wannier Function (MLWF) method.⁷ The coarse mesh grids for electrons and phonons are set as $12 \times 12 \times 12$ and $6 \times 6 \times 6$, respectively. A fine k-mesh grid of

 $40 \times 40 \times 40$ for electron wavevectors is adopted (see the convergence test in the supplementary material), and the q-mesh grid for phonon wavevectors is the same as that for thermal conductivity calculations in the ShengBTE software package, i.e., 25 × 25 × 15. To transform Bloch functions into the MLWF representation, we adopted 18 MLWFs, with initial sp^3 projection for N atom and d projection for Ga atom in the Wannier calculations. Due to the pretty large bandgap of GaN, only valence electron states are considered in EPC. The PBE exchange-correlation functional was selected in Quantum ESPRESSO based calculations, and the optimized normconserving pseudopotential is employed to describe the core-valence interaction,⁸⁰ which also includes the d orbit electrons of Ga atoms in valence electrons. The PAW potential adopted in VASP calculations is not used here in Quantum ESPRESSO calculations since it is not supported by EPW currently. In the following parts, it will be shown that the same selection of exchange-correlation functional is enough to guarantee the consistency optimized lattice constants from different packages, and the difference brought by different pseudopotentials can be negligible. Phonon relaxation time from electron-phonon scatterings will be then added into the phonon relaxation time using the Matthiessen rule.

III. RESULTS AND DISCUSSION

A. GaN structure parameters and strain

Structure relaxation is the first step in first principles calculations. The wurtzite type primitive cell of GaN as shown in Fig. 2 is with a hexagonal system and the P6₃mc space group. The lattice constants *a* and *c*, as well as the internal parameter *u*, are marked in Figs. 2(a) and 2(b), respectively. The *c* axis is also called the polarization axis since there is spontaneous polarization along this axis. In the optimized structure obtained by VASP, the lattice constants are *a* = 3.2188 Å and *c* = 5.2445 Å, and the internal parameter is *u* = 0.3767. These values are larger than experimental values *a* = 3.19 Å and *c* = 5.189 Å⁸¹ by about 1%, which is a normal consequence of PBE functional that will generally overestimate the lattice constants. Since the consistent selection of exchange-correlation



FIG. 2. Schematics of GaN crystal structures: (a) top view, perpendicular to the polarization axis c (in-plane), and (b) side view, along the polarization axis c (cross-plane). The lattice constants a and c, as well as the internal parameter u, are marked.

functional is adopted for calculations in VASP and Quantum ESPRESSO, the lattice constants and internal parameter from Quantum ESPRESSO are almost the same as those from VASP, which are a = 3.2203 Å, c = 5.2458 Å, and u = 0.3767. Basically, there is no standard way to determine the lattice constants when the calculated values are not consistent with those from the experiments. In Lindsay's work,²⁶ the lattice constant from the calculations with the local density approximation (LDA) functional was enlarged by an empirical parameter by 1% for better prediction of phonon dispersion relations, while in Yang's work,²⁸ for consistent setting in VASP and Quantum ESPRESSO, experimental lattice constant values were used in both calculations for consistency of the final results. Though they may provide a better consistency with experimental results in lattice constants and phonon dispersions compared with the original settings, these empirical treatments brought unnecessary artificial factors into the first principles calculations and non-negligible strain in optimized structures. In this work, original lattice constant values are used for all calculations without any artificial adjustments. This makes sense for investigations of the strain effect because an initial structure free of strain is needed. Since the same exchange-correlation functionals are used in VASP and Quantum ESPRESSO packages, optimized lattice constants are nearly the same with only a slight difference smaller than 0.1%. To further verify the consistency between VASP and Quantum ESPRESSO calculations, we also confirmed that electron band structures and phonon dispersion relations from both approaches are almost the same under different strain states (see the supplementary material).

In practical applications of HEMTs, two kinds of strain can be applied on GaN films, i.e., in-plane biaxial strain perpendicular to the polarization axis and cross-plane uniaxial strain along the polarization axis. For the sake of calculation resources and considering that in-plane stress is much more common than cross-plane stress in HEMTs, only biaxial strain effect is investigated in this work. Here, the strain is applied by changing the lattice constants of the structure. The structure is then relaxed with lattice constant a being settled. The biaxial strain is expressed by the relative variation of lattice constant,

$$\sigma_{\rm a} = \frac{a - a_0}{a_0}.$$
 (2)

Similarly, the structure under uniaxial strain is also obtained with the lattice constant c being settled and the uniaxial strain is determined by

$$\sigma_{\rm c} = \frac{c - c_0}{c_0}.\tag{3}$$

Under in-plane (cross-plane) biaxial strain states, the other lattice constant c (a) and internal parameter u will also change for zero stress and the final optimized structures in the cross-plane (in-plane) direction. As shown in Fig. 3, a relative variation of the lattice constant c (a) and internal parameter u changes continuously and nearly linearly with the lattice constant a (c), where the changes of the internal parameter u, defined in the same way as σ_a and σ_c , are very small. Also, it is noted here that changes of the





FIG. 3. Relative variation of lattice constants (black dots) and internal parameter (red dots) under the (a) biaxial strain state and (b) uniaxial strain state.

lattice structure and crystal symmetry are not detected under strain states in this work, i.e., GaN is still in a wurtzite structure with the space group P6₃mc. This also corresponds to the condition in real devices where the lattice structure of GaN is wurtzite type. Consequently, phonon properties as well as the thermal conductivity of GaN are promising to change continuously under strain states from -5% to 5%. In-plane biaxial strain is applied with $\sigma_a = -5\%$ and 5% in final thermal conductivity and EPC calculations.

B. Phonon properties and lattice thermal conductivity

First, we pay attention to the phonon properties and lattice thermal conductivity of GaN in the free state. Figures 4 and 5 show the phonon properties including phonon dispersion relations, phonon DOS, and lattice thermal conductivity with respect to the temperature. The calculated dispersion relation agrees well with those in previous studies^{26–29} and experiments,⁸¹ while a slight difference exits in the absolute values of high-frequency optical phonon branches. This difference is expected to be a consequence of the inconsistency of lattice constants between the calculated and



FIG. 4. (a) Phonon dispersion relations of GaN from calculations by VASP (black dots) and the experiment (hollow dots) from Ref. 81. (b) The total and projected phonon density of states.

experimental values, i.e., overestimated lattice constants (with PBE) may lower the phonon dispersions, while underestimated ones (with LDA) will shift them. As discussed in Sec. III A, the lattice constants used here are a little larger than those from the experiments. For GaN, there are three acoustic phonon branches and nine optical phonon branches, which can be distinguished easily from the dispersion relations where frequencies of acoustic phonon approach to zero at the gamma point. The optical phonon branches, i.e., the other nine phonon branches, can be further divided into two groups according to their frequency magnitude, which are low-frequency optical phonons (three branches) and high-frequency optical phonons (six branches). High-frequency optical branches are sensitive to this inconsistency, while acoustic branches are not, as shown in Fig. 4. The phonon dispersion, as well as phonon density of state, shows several important characteristics. First, the frequency gap between high-frequency optical



FIG. 5. Converged and RTA based lattice thermal conductivities of GaN under the free state with the temperature in the range of (a) 50–500 K and (b) 250–350 K.

phonons and low-frequency branches including acoustic and lowfrequency optical branches is pretty large (~5 THz), and this benefits thermal transport by suppressing $LA + LA/TA \leftrightarrow TO/LO$ phonon scattering channels. Second, the dispersion relation of high-frequency optical branches is nearly flat, which result in highfrequency optical phonons contributing little to phonon thermal transport, and electron-phonon interaction matrix diverges at a long wavelength limit, which will be discussed below. Another characteristic is the splitting of LO-TO phonons illustrated by the splitting and noncontinuity at the gamma point in the phonon dispersion relation. This is a typical characteristic of a polar (ionic) crystal where macroscale periodic electric fields are trigged by polarized longitudinal optical phonons. Figure 4(b) also depicts the projected phonon density of states. It can be seen that Ga atoms mainly contribute to low-frequency phonons (especially acoustic phonons) while N atoms contribute to high-frequency optical phonons.

calculated to be 263 and 259 W/mK for in-plane and cross-plane directions, respectively, as shown in Fig. 5, which are lower than those reported in previous studies. As has been introduced, thermal conductivities calculated by first principles calculations in previous studies are 400/385 W/mK (in-plane/cross-plane),²⁰ 390 W/mK (in-plane),²⁷ 374/420 W/mK (in-plane/cross-plane),²⁸ and 335/317 W/mK (in-plane/cross-plane).²⁹ The difference among the data in this work and those in the literature can be attributed to the following reasons: (1) Ga_d pseudopotential is chosen here with d orbit electrons being treated as valence electrons. This choice is actually suggested from the VASP manual and validated by Yang *et al.*²⁸ as mentioned in Sec. II. (2) Based on the convergence test in this work and Ref. 28, a large supercell size $(5 \times 5 \times 3)$ and the 5th nearest neighbor cutoff distance are needed for third order force constant calculations. (3) Optimized lattice constants are directly used in further calculations without unnecessary artificial adjustments. This work differs from Refs. 26 and 27 in the first and third choices and differs from Ref. 29 in the second choice. Actually, the three choices lead to the difference in the final results. Comparing the case with a normal Ga pseudopotential and a small supersize, our thermal conductivity value is lower. In our separate calculations, the in-plane and cross-plane thermal conductivity are 379 and 391 W/mK, respectively, with normal Ga pseudopotential and a $5 \times 5 \times 3$ supercell, which is much consistent with those from Ref. 28. The convergence test confirms that the thermal conductivity converges when the supercell size increases to $5 \times 5 \times 3$ and the 5th near neighbor atoms are considered, which explains the difference between the results in this work and those in Ref. 29. For the third choice, we have discussed partially in the above part of this section, and the effect of adjusting lattice parameters will be further discussed below. The lattice constants from the optimized structure with the PBE functional are generally lower than experimental values and, therefore, PBE functional based calculations may underestimate the thermal conductivity to some degree, which can explain that the calculation values in this work are a little smaller than the maximum value (280 W/mK) from experiments. In the following, we focus our attention on phonon property analyses and strain effects on lattice thermal conductivity. The calculations and discussions are all built on these bases.

Thermal conductivity of GaN at room temperature is

In Fig. 5, both converged thermal conductivity and thermal conductivity under single relaxation time approximation (RTA) are shown, where the thermal conductivity under RTA can be regarded as the zero-order approximation of Eq. (1). As it is generally acknowledged that RTA is just an appropriate approximation for a phonon resistive process and fails in describing a phonon normal process, we can estimate the contribution of a phonon normal process to thermal conductivity from the difference between converged thermal conductivity and thermal conductivity under RTA. As illustrated in Fig. 5, thermal conductivity under RTA is close to the converged thermal conductivity at a temperature larger than 150 K. The difference is less than 10% at a temperature near 300 K, which confirms that a phonon normal process can be neglected in thermal conductivity calculations based on phonon BTE at room temperature and RTA is still a good approximation for GaN. Figure 6 provides a quantitative description on the distribution of



FIG. 6. Cumulative lattice thermal conductivity of GaN with respect to (a) phonon frequency (dotted lines refer to the phonon frequency where dimensionless cumulative thermal conductivity reaches 90%. Blue, black, and red lines are for the + 5% strain, free, and -5% strain states respectively) and (b) phonon free path under different strain states.

thermal conductivity with phonon frequency and free path. The contribution from phonons with frequency less than 10 THz (acoustic phonons and low-frequency optical phonons) is more than 98% while the contribution from high-frequency optical phonons can be neglected. Specifically, more than 90% thermal conductivity is attributed to phonons with frequency less than 6.4 THz. Figure 6(b) shows that the phonon free path is up to 2.1 μ m when dimensionless cumulative thermal conductivity reaches 90% and mainly ranges from 100 to 2000 nm under the free state, which is quite large and supposed to bring about a strong size effect in thin GaN films.

Now, we turn our attention to strain effects on lattice thermal conductivity. From a classical and intuitional perspective, compressive strain will increase the thermal conductivity as it will increase the elasticity modulus and acoustic velocity. In this work, the results show that not only the absolute value of thermal conductivity changes but also the anisotropy under the strain state changes, which are illustrated comprehensively in Fig. 7. As we can see from Fig. 7(a), lattice thermal conductivity decreases monotonously from 100 to 500 K. Particularly, lattice thermal conductivity at 300-400 K is presented in Fig. 7(b), as the working temperature of GaN-based devices is commonly contained in this section. At room temperature, both in-plane and cross-plane thermal conductivity of GaN decrease remarkably under the +5% strain state (tensile), the average thermal conductivity decreases by 63%, and thermal conductivity shows obvious anisotropy, i.e., cross-plane thermal conductivity is larger than in-plane thermal conductivity. Under the -5% strain state (compressive), average thermal conductivity increases by 53%, and the anisotropy is opposite to that under tensile strain state as in-plane thermal conductivity is larger than the cross-plane part. From a 300-400 K temperature range, lattice thermal conductivity decreases significantly, and the decrease/increase by strain is nearly constant (around 50%) at different temperatures. Actually, the changes of lattice thermal conductivity under the strain state are comparable to or even larger than those caused by temperature changes (300-400 K). Furthermore, temperature dependence of thermal conductivity follows the same tendency under different strain states in general. Also, low-frequency phonons still contribute the most part to thermal conductivity, which is larger than 97%.

Figure 8 demonstrates the changes of phonon dispersion relations and DOS under different strain states. Acoustic phonon branches are not sensitive to strain, and phonon frequency only increases/decreases slightly under the compressive/tensile strain state. Opposite to acoustic phonons, the phonon dispersion relation of high-frequency optical phonons shows obvious increase/decrease of phonon frequency under the compressive/tensile strain state. According to the results of phonon DOS in Fig. 8(b), the phonon bandgap between the highest frequency phonons in the lower part and the lowest frequency phonons in the higher part (similar to the bandgap in the electron band structure) can be obtained, which are 2.2263, 3.1152, and 3.8020 THz under tensile strain, free, and compressive strain state, respectively. Since a large phonon bandgap will suppress the three-phonon scattering processes where two acoustic phonons combine into an optical phonon, it will decrease the scattering rates of low-frequency phonons. In particular, dimensionless cumulative thermal conductivity with respect to phonon frequency and free path under different strain states are shown in Fig. 6. Consistent with phonon dispersion relations under different strain states, phonons with lower/higher frequency contribute more to lattice thermal conductivity under the tensile/compressive strain state. Phonons' frequency decreases to 6.2 THz when dimensionless cumulative thermal conductivity reaches 90% under the tensile strain state, while it increases to 7.1 THz under the compressive strain state. Following the discussion on phonon free path as depicted by Fig. 6(b) in the above paragraph, the size effect will become stronger under compressive strain state while it weakens under the tensile strain state. In detail, the phonon free path is as long as $3.7 \,\mu m$ when dimensionless cumulative thermal conductivity reaches 90% and mainly ranges from 150 to 4000 nm under the



FIG. 7. Lattice thermal conductivity in the temperature range of (a) 100–500 K and (b) 300–400 K. (c) Lattice thermal conductivity of GaN at room temperature under different strain states.

compressive strain state. Under the tensile strain state, the phonon free path decreases to $1.2\,\mu$ m for 90% dimensionless cumulative thermal conductivity and mainly ranges from 40 to 1500 nm. It is noted here that the lattice thermal conductivity and phonon



FIG. 8. (a) Phonon dispersion relations and (b) phonon density of states under different strain states.

dispersion relation are sensitive to strain, which further confirms that different treatments on optimized lattice constants lead to a significant difference on the lattice thermal conductivity and phonon dispersion relation.

Based on the phonon BTE, thermal conductivity can be expressed as

$$\boldsymbol{\kappa}_{L}^{\alpha\beta} = \sum_{\mathbf{q}\nu} c_{\nu,\mathbf{q}\nu} v_{\mathbf{q}\nu}^{\alpha} v_{\mathbf{q}\nu}^{\beta} \tau_{\mathbf{q}\nu}, \tag{4}$$

in which $c_{\nu,\mathbf{q}\nu}$ is the volume specific heat of phonon mode \mathbf{q}, ν . Then, it is clear that thermal conductivity depends on specific heat, phonon group velocity, and relaxation time directly. In the following, we will show the changes of these three physical quantities under different strain states. In Fig. 9(a), scattering rates increase under the tensile strain state and decrease under the compressive strain state, which is consistent with the changes of the phonon



FIG. 9. (a) Phonon-phonon scattering rates, (b) Grüneisen parameters, (c) specific heat, and (d) group velocity under different strain states.

bandgap above. Besides, the increase/decrease of scattering rates under the tensile/compressive strain also results from the increase/ decrease of anharmonicity, as illustrated in Fig. 9(b), where Grüneisen parameters increase/decrease under the tensile/compressive strain



state. Figures 9(c) and 9(d) mainly show the phonon harmonic properties under different strain states. Specific heat reflects the energy level of the crystal system and changes with the change of phonon dispersion relation correspondingly. Under strain states, the changes of specific heat are less than 3%, which is supposed to contribute little to changes of thermal conductivity. Under the compressive strain state, both phonon group velocity and specific heat increase, which is consistent with the increased thermal conductivity. Obviously, with the consistent changes of phonon scattering rates, specific heat and group velocity shown in Figs. 9(a), 9(c) and 9(d), lattice thermal conductivity will change remarkably. To have a quantitative understanding on lattice thermal conductivity changes under strain states, we perform the analyses on changes of thermal conductivity at restricted conditions. In Fig. 10(a), "Relaxation time," "Group velocity," and "Specific heat" are marked as restricted conditions, e.g., "Relaxation time" means that only the relaxation time under the +5% strain state is used, while group velocity and specific heat under free state are used for calculation of thermal conductivity under the +5% tensile strain state. These changes of lattice thermal conductivity at restricted conditions are compared with the real changes under the strain state marked as "Real." As illustrated in Figs. 10(a) and 10(b), the changes of thermal conductivity at the "Relaxation time" restricted condition can be as large as 90% of the real changes under the tensile strain state and around 60% under the compressive strain state. The comparisons among three restricted conditions depict that relaxation time (scattering rates) is the most important physical quantity for changes of lattice thermal conductivity under strain states while contribution from specific heat is very small, especially for the tensile strain state condition. For the compressive strain state condition shown in Fig. 10(b), contribution from relaxation time and group velocity are comparable.

Based on the thermal conductivity formula, the anisotropy of lattice thermal conductivity mainly comes from the anisotropy of squared phonon group velocity. In Fig. 11, we particularly



FIG. 10. Changes of lattice thermal conductivity at restricted conditions under (a) the +5% tensile strain state and (b) the -5% compressive strain state.

show the squared phonon group velocity in in-plane and crossplane directions with respect to the phonon frequency. Since lattice thermal conductivity is mainly attributed to acoustic phonons and low-frequency optical phonons, we focus on phonons with frequency in the range of 0-10 THz. From the comparison between Figs. 11(a) and 11(b), it is found that in-plane squared phonon group velocity shows more sensitive response to strain than cross-plane squared group velocity, as more red/blue dots are located on the top/bottom of black dots under the compressive/tensile strain state for in-plane squared group velocity. Theoretically, the cross-plane uniaxial strain resulting from the in-plane biaxial strain will be suppressed by the induced piezoelectric polarization. As a consequence, the effect of strain on the cross-plane lattice thermal conductivity may be weakened, i.e., changes of cross-plane thermal conductivity are a little smaller than those of in-plane thermal conductivity, which then results in the changes of anisotropy of lattice thermal conductivity under different strain states.



FIG. 11. Squared (a) in-plane and (b) cross-plane phonon group velocity.

C. Contribution from electron-phonon coupling

As mentioned above, a Fröhlich-type electron-phonon interaction is important in polar materials where electrons can couple strongly with the macroscopic electric fields generated by the longitudinal optical phonons at long wavelengths.⁷⁸ The nontrivial contribution from a Fröhlich EPC to lattice thermal conductivity of GaN has been confirmed in Yang's work.²⁸ Here, we further discuss the strain effects on EPC and how the role of EPC changes under strain states in lattice thermal conductivity.

Strictly speaking, the electron-phonon scattering process is an inelastic scattering process for phonons. Hence, relaxation time approximation may be limited to reflect the role of electronphonon interactions in lattice thermal transport. However, this handling method is still constructive to describe the effects of EPC on the lattice thermal transport. Under relaxation time approximation, it is simple to take EPC into consideration in lattice thermal conductivity calculations using the Matthiessen rule,

$$\frac{1}{\tau_{qv}} = \frac{1}{\tau_{qv}^{ph}} + \frac{1}{\tau_{qv}^{e-ph}},$$
(5)

where the total scattering rates are the sum of scattering rates from phonon-phonon scatterings and electron-phonon scatterings. In the calculations for EPC, the bandgaps under three different states are checked, which are 1.76 eV, 1.11 eV, and 1.82 eV for the free, tensile strain, and compressive strain states, respectively. It has been known and confirmed that density functional theory will underestimate the bandgap significantly;^{50,77} in other words, the bandgap of GaN under strain states is still large enough to ignore the thermal excitation. Therefore, the assumption that only valence electron states are considered in EPC, as mentioned in Sec. II, is still adopted here for calculations under strain states. Besides, for saving resources, only EPC at the room temperature is calculated. Figure 12 presents these two kinds of phonon scattering rates under different strain states. In all the three cases with different strain states, the highest electron-phonon scattering rates are comparable with phonon-phonon scattering rates, especially for phonons at a high frequency. Actually, despite that EPC is large for high-frequency phonons, the influence of EPC with high phonon frequency on thermal transport is very small since highfrequency phonons have little contribution to thermal transport. Hence, the decrease of thermal conductivity mainly results from the EPC with phonon frequency below the gap. Under strain states, electron-phonon scattering rates change in both absolute and relative values. Specifically, electron-phonon scattering rates under tensile strain state decrease a lot compared with those under free and compressive strain states, while electron-phonon scattering rates show a little increase and are still comparable with those under the free state. Theoretically, electron-phonon scattering rates depend on phonon energy, electron DOS near the Fermi level, i.e., in the Fermi window, and electron-phonon coupling matrix element.^{78,82} The higher the three terms, the larger the scattering rates. Phonon frequency, which has been discussed in Sec. III B, implies that compressive strain may result in larger electron-phonon scattering rates since it increases the phonon frequency. The electron DOS in the Fermi window (4 eV in this work) under different strain states are present in Fig. 13. In different energy ranges, the largest electron DOS corresponds to different strain states. Since electron states within 1 eV near the Fermi level contribute the most, the results illustrate that there are larger scattering rates for the free state condition. Electron-phonon coupling is represented by the total electron-phonon coupling strength λ , which basically represents a combined result from electron DOS and electron-phonon coupling matrix,70

$$\lambda = \sum_{\mathbf{q}\nu} \frac{1}{N(\varepsilon_{\mathrm{F}})} \sum_{nm} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{\Omega_{\mathrm{BZ}}} \times |g_{mn,\nu}(\mathbf{k},\mathbf{q})|^2 \delta(\varepsilon_{n\mathbf{k}} - \varepsilon_{\mathrm{F}}) \delta(\varepsilon_{m\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathrm{F}}),$$
(6)

where N is the electron distribution function, g is the electronphonon coupling matrix, and ε is the energy of electron. BZ, **k**, **q**, and F represent the Brillouin zone, the electron wave vector, the



FIG. 12. Phonon-phonon scattering rates and electron-phonon scattering rates under different strain states: (a) free state, (b) +5% strain state, and (c) -5% strain state.



FIG. 13. Electron density of states of GaN for valence band in the Fermi window (4 eV) under different strain states.

phonon wave vector, and the Fermi level, respectively. For free, tensile strain, and compressive strain states, λ is 1.23, 1.35, and 0.92, respectively. As we can see from Figs. 12(a)–12(c), phonon scattering rates from EPC under free and compressive strain states are obviously smaller. However, changes of phonon frequency and electron-phonon coupling strength are not consistent. To sum up, nearly unchanged phonon scattering rates from EPC under compressive strain states are strain states results from a competition mechanism between the increase of phonon frequency and the decrease of phonon scattering rates from EPC under the tensile strain state is mainly the consequence of lower phonon frequency despite that the electron-phonon coupling strength is larger.

In Fig. 14, we show the comparison among lattice thermal conductivities with and without considering the contribution from EPC under different strain states. According to the changes of lattice thermal conductivity, we can evaluate the role of EPC in lattice thermal conductivity. Under strain states, the changes of lattice thermal conductivity including contribution from EPC are around 60%, compared with those not including the contribution from EPC. Decreases of lattice thermal conductivities in both in-plane and cross-plane directions due to the EPC are obviously different. Concretely speaking, the decreases are 25.8% and 26.9% under the free state for in-plane and cross-plane directions, respectively. The decreases under the -5% strain state are nearly the same as those under the free state, i.e., 19.5% and 23.5% for in-plane and cross-plane directions, but these are small under the +5% strain state, i.e., 7.2% and 4.6% for in-plane and cross-plane directions. Furthermore, electron-phonon scattering rates decrease under the tensile strain state (especially for the low-frequency part), and meanwhile, phonon-phonon scattering rates increase. Therefore, the contribution from EPC to lattice thermal conductivity decreases remarkably under the tensile strain state. For



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FIG. 14. Lattice thermal conductivity with and without including contribution from EPC at room temperature.

the case under the compressive state, electron-phonon scattering rates nearly keep unchanged with a slight decrease and phonon-phonon scattering rates decrease. The final result is that the decrease of lattice thermal conductivity as well as the role of EPC are comparable with that under the free state. Basically, this is the result of combined effects from decreased phonon-phonon scattering rates, nearly constant electron-phonon scattering rates, and the absolute value of lattice thermal conductivity without EPC. From the perspective of absolute values, decreases of lattice thermal conductivity in absolute value under the -5% strain state are 78 and 91 W/mK for in-plane and cross-plane conditions, larger than those under the free state, 68 and 69 W/mK, respectively. Since the EPC does not affect the phonon group velocity and frequency of dominant phonons nearly keeps unchanged, the anisotropy of lattice thermal conductivity including the contribution from EPC is preserved.

It is noted here that the lattice thermal conductivity of GaN including the contribution from EPC is lower than the maximum experimental values. As we directly select the optimized lattice constants without artificial adjustment, which are larger than the experimental data, this may lead to the lower thermal conductivity partially. Meanwhile, EPC is taken into consideration simply using the Matthiessen rule, which may not be accurate enough in describing the lattice thermal transport including the contribution from EPC, since the electron-phonon scattering process is an inelastic process for phonons. Further discussion is beyond the scope of this research and will be carried out in future work.

IV. CONCLUSIONS

Using the first principles calculation method and on the basis of a careful selection of important parameters (pseudopotential, supercell size) and the determination of lattice constants, lattice thermal conductivity of GaN including the contribution from EPC is investigated under three different in-plane biaxial strain states, i.e., free state, tensile strain state, and compressive strain state. At a range of strain from -5% to +5%, the lattice structure and crystal symmetry of GaN are preserved. The lattice thermal conductivity changes monotonously and remarkably under strain states, i.e., it decreases under the tensile strain state and increases under the compressive strain state, which is mostly attributed to the changes of phonon relaxation time. The anisotropy of lattice thermal conductivity is weak under the free state, while it becomes larger under the strain states. Under the tensile strain state, cross-plane lattice thermal conductivity is larger than cross-plane thermal conductivity, while it is opposite under the compressive strain state. This difference in anisotropy, shown by different changes of squared in-plane and cross-plane group velocity, may be a consequence of the weakening effect from strain induced polarization, which screens the strain effects partially.

The lattice thermal conductivity of GaN including the contribution from EPC under different strain states is calculated in this work. Under strain states, the decrease of lattice thermal conductivity is around 60%, which is comparable to those not including contribution from EPC. The decrease of lattice thermal conductivity when the contribution from EPC is taken into consideration differs for different strain states. Under the compressive strain state, the decreases of lattice thermal conductivity are 19% and 23% for the in-plane and cross-plane conditions, respectively, comparable with those under the free state. The decreases are small under the tensile strain state, especially for the cross-plane condition, due to the increase of phonon anharmonicity and decrease of electron-phonon scattering rates. The anisotropy of lattice thermal conductivity including the contribution from EPC is still the same as that without including EPC.

Nowadays, substrates, such as sapphire, MgO, SiC, ZnO, and Si, have been technically available for GaN. Based on a detailed lattice mismatch, ZnO and Si can be classified as the compressive strain group since their lattice constants are larger than those of GaN, while sapphire, MgO, and SiC can be classified as the tensile strain group. The results in this work show that in-plane biaxial strain plays an important role in thermal transport as it affects both the absolute value and the anisotropy of thermal conductivity as well as the role of EPC in lattice thermal transport. Therefore, thermal performance of GaN-based devices depends on the selection of substrates, which will significantly affect the temperature distribution and hot spot temperature in real devices.

SUPPLEMENTARY MATERIAL

See the supplementary material for (i) electron band structures and phonon dispersion relations from VASP and Quantum ESPRESSO under different states and (ii) the convergence test for *k*-mesh in electron-phonon coupling calculations.

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