Influence of surface scattering on the thermal properties of spatially confined GaN nanofilm*

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Gallium nitride (GaN), the notable representative of third generation semiconductors, has been widely applied to optoelectronic and microelectronic devices due to its excellent physical and chemical properties. In this paper, we investigate the surface scattering effect on the thermal properties of GaN nanofilms. The contribution of surface scattering to phonon transport is involved in solving a Boltzmann transport equation (BTE). The confined phonon properties of GaN nanofilms are calculated based on the elastic model. The theoretical results show that the surface scattering effect can modify the cross-plane phonon thermal conductivity of GaN nanostructures completely, resulting in the significant change of size effect on the conductivity in GaN nanofilm. Compared with the quantum confinement effect, the surface scattering leads to the order-of-magnitude reduction of the cross-plane thermal conductivity in GaN nanofilm. This work could be helpful for controlling the thermal properties of GaN nanostructures in nanoelectronic devices through surface engineering.

Keywords: GaN nanofilm, elastic model, quantum confinement, Boltzmann transport equation, size effect, phonon thermal conductivity

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1. Introduction

Semiconductor nanostructures have received a great deal of attention due to their improved material properties, which are quite different from those of their bulk counterparts. Since GaN nanostructures have prominent and enhanced physicochemical properties at high temperatures,[1–6] its nanostructured elements such as nanowires, nanofilms and nanotubes, have been widely studied and used in nanoelectronic devices,[7,8] such as high-electron-mobility transistors (HEMTs),[9] light-emitting diodes (LEDs),[10] and biochemical sensors.[11,12] However, the increase of temperature from heat generation makes the heat dissipation significantly difficult in devices, leading to a sharp decline in material properties of GaN-based nanodevices. Therefore, how to improve the phonon thermal conductivity of GaN nanostructures has currently become a major challenge in keeping the performance and reliability of GaN nano-electronic devices.

The thermal conductivity of GaN nanostructures has been extensively investigated since the first GaN-based transistor was generated in 1998. For example, Balandin *et al.*[13] proposed a new concept of phonon engineering to control the thermal properties of GaN-based nanostructures and pave the way for future ground-breaking development in nanoelectronic devices. Wang *et al.*[14] calculated the thermal conductivity of GaN nanowires by applying non-equilibrium atomistic simulation methods. Coincidentally, Guthy *et al.*[15] prepared GaN nanowires with diameters varying from 97 nm to 181 nm, grown by thermal chemical vapor deposition (CVD), and measured the thermal conductivity in a range of 13 W/m·K–19 W/m·K at 300 K. Zou[16] used the Boltzmann transport equation (BTE) to predict the lattice thermal conductivity of GaN nanowires. Zhou and Li[17] also calculated the phonon thermal conductivity of GaN nanotubes based on the BTE. In addition to the elastic continuum models and BTE, first principles and molecular dynamics simulations were also utilized to analyze the lattice thermal conductivities of GaN bulks and nanostructures.[18–21] Moreover, the influences of certain dopant or crystal defects on the phonon properties and thermal properties of GaN have been analyzed in detail.[22–24] Zhu and Ruan[25] further investigated the effect of a prestress field on the thermal conductivity of GaN nanostructures. The effect of a built-in-polarization field on the thermal conductivity of GaN nanostructure was also studied.[26,27] On the other hand, some work has been done to explore the thermal transports in the semiconductors and thermal management of stretchable inorganic electronics.[28–30] However, quantitative understandings of the surface effect and quantum confinement effect on the thermal properties of GaN nanostructures are lacking in the literature.

In this work, the quantum confinement effect and surface scattering effect are taken into account in simulating the thermal conductivity of GaN nanofilm. The elastic model is addressed to describe the confinement effect on phonon properties of GaN nanofilm. The BTE approach is used to analyze

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the contribution of surface scattering to the phonon transport in the GaN nanofilm. The calculations demonstrate that the surface scattering effect leads to the more significant size effect on the thermal conductivity of GaN nanofilm. The dependences of the temperature and parameters on the conductivity are also analyzed in detail.

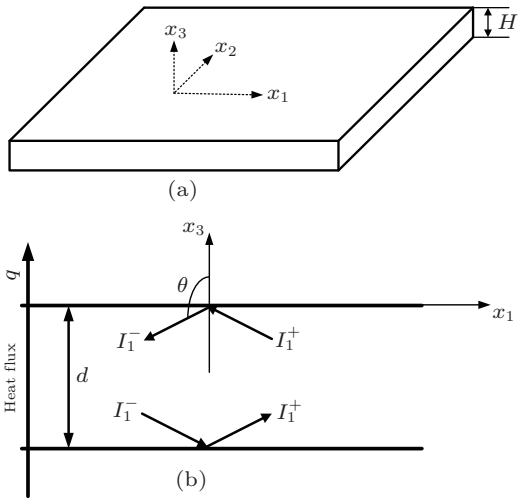


Fig. 1. Schematic diagram of a GaN nanofilm (a) and surface phonon scattering (b).

2. Theoretical model

2.1. Continuum elasticity theory

The continuum elasticity theory is often utilized to characterize the acoustic phonon properties of spatially confined GaN nanostructures.[31–33] The free-standing monolayer GaN nanofilm is supposed to be the isotropic material in its natural state as shown in Fig. 1(a). Here, x_1 and x_2 denote the in-plane directions and x_3 refers to the transverse direction. The vibration governing equation in the framework of elasticity theory is expressed as[28,34]

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j}. \tag{1}$$

Here, u_i is the displacement vector, ρ is the density, σ_{ij} is the elastic stress tensor which can be written as

$$\sigma_{ij} = C_{ijkl} u_{kl}, \tag{2}$$

where C_{ijkl} is the natural second-order elastic constant, and the strain tensor is given by

$$u_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \tag{3}$$

When the lattice wave propagates along the x_1 direction, the displacement of the nanofilm is the function of x_1 and x_3. The solutions for the displacement of Eq. (1) can be easily given in the form of

$$\boldsymbol{u} = \hat{\boldsymbol{u}}(x_3)\exp\left[\mathrm{i}(\omega t - q_0 \cdot x_1)\right], \tag{4}$$

where ω is the phonon frequency, q_0 is the wave vector, and $\hat{\boldsymbol{u}}$ is the amplitude of displacement vector. Substituting Eq. (4) into Eq. (1), the corresponding eigenvalue equation can be written as

$$\boldsymbol{D}\hat{\boldsymbol{u}}(x_3) = -\rho\omega^2 \hat{\boldsymbol{u}}(x_3), \tag{5}$$

where

$$\boldsymbol{D} = \begin{bmatrix} C_{44}\dfrac{\mathrm{d}^2}{\mathrm{d}x_3^2} - C_{11}q_0^2 & 0 & -\mathrm{i}q_0(C_{13}+C_{44})\dfrac{\mathrm{d}}{\mathrm{d}x_3} \\ 0 & C_{44}\dfrac{\partial^2}{\partial x_3^2} - C_{66}q_0^2 & 0 \\ -\mathrm{i}q_0(C_{13}+C_{44})\dfrac{\mathrm{d}}{\mathrm{d}x_3} & 0 & C_{33}\dfrac{\mathrm{d}^2}{\mathrm{d}x_3^2} - C_{44}q_0^2 \end{bmatrix}. \tag{6}$$

According to the classic acoustic theory,[35] there are three kinds of phonon confinement modes, i.e., the shear mode (SH), the dilatational mode (SA), and the flexural mode (AS). For the SH mode, one can substitute the solution $u_2 = \hat{u}_2(x_3)\exp\left[\mathrm{i}(\omega t - q_0 \cdot x_1)\right]$ into Eq. (5) to obtain the eigenvalue equation as

$$C_{44}\frac{\mathrm{d}^2\hat{u}_2}{\mathrm{d}x_3^2} + \left[\rho\omega^2 - C_{66}q_0^2\right]\hat{u}_2 = 0. \tag{7}$$

For the SA and AS modes, the corresponding eigenvalue equations could be expressed as

$$\begin{cases} C_{44}\dfrac{\mathrm{d}^2\hat{u}_1}{\mathrm{d}x_3^2} - \mathrm{i}q_0(C_{13}+C_{44})\dfrac{\mathrm{d}\hat{u}_3}{\mathrm{d}x_3} + \left[\rho\omega^2 - C_{11}q_0^2\right]\hat{u}_1 = 0, \\ C_{33}\dfrac{\mathrm{d}^2\hat{u}_3}{\mathrm{d}x_3^2} - \mathrm{i}q_0(C_{13}+C_{44})\dfrac{\mathrm{d}\hat{u}_1}{\mathrm{d}x_3} + \left[\rho\omega^2 - C_{44}q_0^2\right]\hat{u}_3 = 0. \end{cases} \tag{8}$$

The boundary conditions of free-standing nanofilm for three independent phonon modes can be expressed as

$$\begin{cases} \sigma_{23} = \dfrac{\partial u_2}{\partial x_3} = 0, & \text{(9a)} \\ \sigma_{13} = \dfrac{\partial u_1}{\partial x_3} - \mathrm{i}q_0 u_3 = 0, \\ \sigma_{33} = C_{33}\dfrac{\partial u_3}{\partial x_3} - \mathrm{i}q_0 C_{13} u_1 = 0. & \text{(9b)} \end{cases}$$

Here, the boundary condition in Eq. (9a) is utilized to calculate the dispersion relation for SH mode, and the boundary conditions in Eq. (9b) are for the SA and AS modes. Combining the corresponding boundary conditions in Eq. (9a) with Eqs. (7) and (8), the dispersion relation of each mode can be figured out through the finite element difference method.

According to the phonon dispersion relations of various modes derived from the above equations for the semiconductor nanostructures, the phonon group velocity v_n for the n-th branch of phonon modes can be solved by $v_n(q) = \mathrm{d}\omega_n(q)/\mathrm{d}q$, where ω_n and q denote the phonon frequency and the phonon wave vector, respectively. Based on Callaway's model, the frequency-dependent average phonon group velocity can be expressed as[36]

$$\bar{V} = \left\{ \frac{1}{m(\omega)} \sum_{N=1}^{M(\omega)} \left[v_n^{\mathrm{SA,AS,SH}}(\omega) \right]^{-1} \right\}^{-1}, \tag{10}$$

where the superscripts SA, AS, SH are the types of polarization, the subscript n is the quantum number of the modes for a particular wave vector, and m is the number of the total phonon branches. The quasi-two-dimensional (2D) phonon density of state (DOS) can be given as

$$f_n^{\mathrm{SA,AS,SH}}(\omega) = (1/2H\pi) q_n^{\mathrm{SA,AS,SH}}(\omega) / v_n^{\mathrm{SA,AS,SH}}(\omega),$$

where H is the nanofilm thickness. The total DOSs for all polarizations calculated by a summation over all n's can then be given by[36]

$$F^{\mathrm{SA,AS,SH}}(\omega) = \sum f_n^{\mathrm{SA,AS,SH}}(\omega). \tag{11}$$

2.2. Phonon Boltzmann transport approach

The phonon Boltzmann transport equation (BTE) is a powerful approach to describing the heat energy transports in micro/nanoscale systems,[16,17,37–41] which can be expressed basically as

$$\frac{\partial f}{\partial t} + \boldsymbol{v}\nabla_r f + \dot{\boldsymbol{k}}\nabla_k f = \left(\frac{\partial f}{\partial t}\right)_{\mathrm{s}}, \tag{12}$$

where v is the phonon velocity, k is the wave vector, f is the non-equilibrium phonon distribution function, $(\partial f/\partial t)_{\mathrm{s}}$ is the rate of change of f due to scattering, which is often simplified by the relaxation-time approximation into

$$\left(\frac{\partial f}{\partial t}\right)_{\mathrm{s}} = -\frac{f - f_0}{\tau}. \tag{13}$$

The equation above describes a relaxation process, indicating that if the external field is removed, the phonon distribution function f will return to the equilibrium state f_0. The Bose–Einstein distribution function f_0 can be expressed as

$$f_0(E) = \frac{1}{\mathrm{e}^{(E(\boldsymbol{k})-E_{\mathrm{F}})/k_{\mathrm{B}}T} + 1}, \tag{14}$$

where E is the wave vector-dependent energy level, E_{F} is the Fermi energy, k_{B} is the Boltzmann constant, and T is the temperature. Since the BTE is applicable for describing the phonon transport in the nanofilms, we give it in terms of the total phonon intensity defined as[37,38]

$$I = \frac{1}{4\pi} \sum_m \int_0^{v_{\max}} |V_m| f h v D_m(v)\, \mathrm{d}v, \tag{15}$$

where $|V_m|$ is the magnitude of the phonon group velocity, h is the Planck constant, and D is the density of states per unit volume. When the heat conduction is perpendicular to the plane as shown in Fig. 1(b), the phonon transport equation of the GaN nanofilm under the relaxation-time approximation can be transformed into

$$\sin\theta\cos\phi\frac{\partial I}{\partial x_1} + \sin\theta\sin\phi\frac{\partial I}{\partial x_2} + \cos\theta\frac{\partial I}{\partial x_3} = -\frac{I - I_0}{\Lambda}, \tag{16}$$

where I_0 is the equilibrium phonon intensity acquired by substituting f_0 into Eq. (15) with the Bose–Einstein distribution in Eq. (14), θ and ϕ are the polar and the azimuthal angles, respectively. $\Lambda (= |\boldsymbol{v}|\tau)$ is the average phonon mean free path (MFP). Here, $\boldsymbol{v}$ denotes the phonon velocity, and τ refers to the relaxation time. The phonon diffusion transport across nanofilm can be treated as the phonon radiation transport, and the phonon ballistic transport across the grain boundary can also be treated as a similar thermal radiation.[37]

Due to the surface scattering, the phonon distribution function f only depends on the x_3 direction. As a result, the phonon intensity I is homogeneous in the plane but changes along the x_3 direction. Through introducing a deviation function $i(x_3,\theta) = I(x_3,\theta) - I_0(T)$, the phonon transport equation (16) can be rewritten as

$$\cos\theta\frac{\partial i}{\partial x_3} + \frac{i}{\Lambda} = -\cos\theta\frac{\mathrm{d}I_0}{\mathrm{d}x_3}. \tag{17}$$

The solution of the differential equation above can be easily obtained as

$$\begin{cases} i(\eta,\mu) = i^+(\eta,\mu) = i^+(0,\mu)\,\mathrm{e}^{-\eta/\mu} - \displaystyle\int_0^{\eta} \frac{\mathrm{d}I_0}{\mathrm{d}t}\,\mathrm{e}^{-(\eta-t)/\mu}\,\mathrm{d}t, \quad (0<\mu<1), \\ i(\eta,\mu) = i^-(\eta,\mu) = i^-(\xi,\mu)\,\mathrm{e}^{(\xi-\eta)/\mu} + \displaystyle\int_{\eta}^{\xi} \frac{\mathrm{d}I_0}{\mathrm{d}t}\,\mathrm{e}^{-(\eta-t)/\mu}\,\mathrm{d}t, \quad (-1<\mu<0), \end{cases} \tag{18}$$

where $\mu (= \cos\theta)$ is the directional cosine, $\eta (= x_3/\Lambda)$ the nondimensional $x_3$coordinate, and $\xi (= d/\Lambda)$ the nondimensional thickness.

In order to determine the parameters $i^+(0,\mu)$ and $i^-(\xi,\mu)$, the boundary conditions should be addressed. The surface scattering models can be divided into the totally diffuse scattering surfaces, the totally specular scattering surfaces and the partially diffuse and partially specular scattering surfaces.[39] In this work, the boundary conditions for partially diffuse and partially specular scattering surfaces are involved. The specular scattering fraction p is introduced which represents the fraction of phonons experiencing specular scattering at the surface. Since the nanofilm is monolayer, the energy reflectivity R at the surface should be taken into account. It can be divided into the specular portion R_s and the diffuse portion R_d. The energy transmissivity T is neglected. Therefore, the energy balance can be written as

$$\begin{aligned} I^+(0,\mu) &= p\left[R_s(\mu)I^-(0,-\mu)\right] \\ &\quad +2(1-p)\left[R_d\int_{2\pi} I^-(0,-\mu)\mu\,\mathrm{d}\mu\right], \\ I^-(\xi,-\mu) &= p\left[R_s(\mu)I^+(\xi,\mu)\right] \\ &\quad +2(1-p)\left[R_d\int_{2\pi} I^+(\xi,\mu)\mu\,\mathrm{d}\mu\right]. \end{aligned} \tag{19}$$

Based on Eqs. (18) and (19), the parameters $i^+(\eta,\mu)$ and $i^-(\eta,\mu)$ can be determined. Therefore, the heat flux q along the cross-plane direction of nanofilm can be obtained from[42]

$$\begin{aligned} q(\eta) &= \int_{4\pi} I\cos\theta\,\mathrm{d}\Omega \\ &= 2\pi\int_0^1 \left[i^+(\eta,\mu)-i^-(\eta,-\mu)\right]\mu\,\mathrm{d}\mu, \end{aligned} \tag{20}$$

where $\mathrm{d}\Omega(=2\pi\sin\theta\,\mathrm{d}\theta)$ is the differential solid angle.

2.3. Phonon thermal conductivity

Since the flow stress is along the x_3 direction as shown in Fig. 1(b), the cross-plane thermal conductivity κ_{cp} can be derived from the heat flux q based on the Fourier law as follows:[43]

$$q = -\kappa_{cp}\nabla T, \tag{21}$$

where ∇T is the temperature gradient. Combining Eq. (25) and Eq. (26), the cross-plane thermal conductivity κ_{cp} of GaN nanofilm that is affected simultaneously by the quantum confinement effect and surface scattering effect, can be expressed as

$$\kappa_{cp} = \kappa_1 G_0, \tag{22}$$

where κ_1 is the phonon thermal conductivity accounting for the quantum confinement effect, and expressed as[44]

$$\begin{aligned} \kappa_1 &= \frac{1}{3}\left(\frac{k_B}{\hbar}\right)k_B T\int_{x_{min}}^{x_{max}} \frac{x^2 e^x}{(e^x-1)^2}\tau(x)\bar{V}^2(x)F(x)\,\mathrm{d}x \\ &= \kappa_0 G_1. \end{aligned} \tag{23}$$

Here, $x=\hbar\omega_n(q)/k_B T$, τ is the phonon relaxation time, $\bar{V}$ the average phonon group velocity, F the total density of states (DOSs), and κ_0 the bulk thermal conductivity. Thus, the cross-plane thermal conductivity of nanofilm κ_{cp} can be rewritten as

$$\kappa_{cp} = \kappa_0 G, \tag{24}$$

where $G(=G_0G_1)$ represents the ratio of κ_{cp} to the bulk thermal conductivity κ_0. It is noted that G depends on the surface scattering parameters, the thickness of nanofilm, and temperature.

In general, the phonon scattering mechanisms can be classified as the three-phonon scattering, point-defect scattering, boundary scattering, and phonon-electron scattering. According to the Klemens' second-order perturbation theory, the Umklaap scattering rate at room temperature can be expressed as[45,46]

$$\frac{1}{\tau_U} = 2\gamma^2\frac{k_B T}{\mu V_0}\frac{\omega^2}{\omega_D}, \tag{25}$$

where γ is the Grunieisen anharmonicity parameter, T is the temperature, μ is the shear modulus, V_0 is the volume per atom, and ω_D is the Debye frequency. The point-defect scattering rate suffering the difference of mass between atoms in materials can be given as[47,48]

$$\frac{1}{\tau_M} = \frac{V_0\Gamma\omega^4}{4\pi V^3}, \tag{26}$$

where V is the phonon group velocity, and Γ is the measure of the strength of the point-defect scattering. The relaxation time for the interaction between acoustic phonons and electron at low doping levels is given by[49,50]

$$\frac{1}{\tau_{ph-e}} = \frac{n_e\varepsilon_1^2\omega}{\rho V^2 k_B T}\sqrt{\frac{\pi m^* V^2}{2k_B T}}\exp\left(-\frac{m^* V^2}{2k_B T}\right), \tag{27}$$

where n_e is the concentration of conduction electrons, ε_1 the deformation potential, ρ the mass density, and m^* the electron effective mass. According to the Callaway and Klemens formulation[51,52] the total phonon scattering relaxation time τ follows the Matthiessen rule $\tau^{-1}=\tau_U^{-1}+\tau_M^{-1}+\tau_{ph-e}^{-1}$.

3. Results and discussion

To give an insight into the influences of the surface scattering effect and quantum confinement effect on the phonon thermal conductivity of GaN nanofilms with various film thickness and different temperatures, the numerical calculations for the wurtzite structured GaN nanofilms under the SH mode will be presented as an example. The elastic modulus of bulk GaN are $C_{33}=252$ GPa, $C_{13}=129$ GPa, $C_{44}=148$ GPa.The other parameters are selected in Refs. [16], [53]–[55].

In view of the derivation of the phonon dispersion relation, the phonon properties of GaN nanofilms, such as phonon group velocity and phonon density of states (DOS) can be calculated. Figure 2 shows the phonon properties of SH mode

for GaN nanofilm, in which the nanofilm thickness is 3.19 nm. The phonon group velocity as a function of the wave vector is shown in Fig. 2(a). It is noted that the slopes of phonon group velocity for each order become smaller with the increase of the wave vector, and then all curves become flat to approach to a limit value, namely the transverse wave velocity of the nanofilm. Figure 2(b) shows the DOS of SH mode as a function of phonon energy. It is clearly found that there exits an oscillatory behavior of the DOS and each step corresponds to the oncoming of new phonon branches due to the quantum confinement effect.

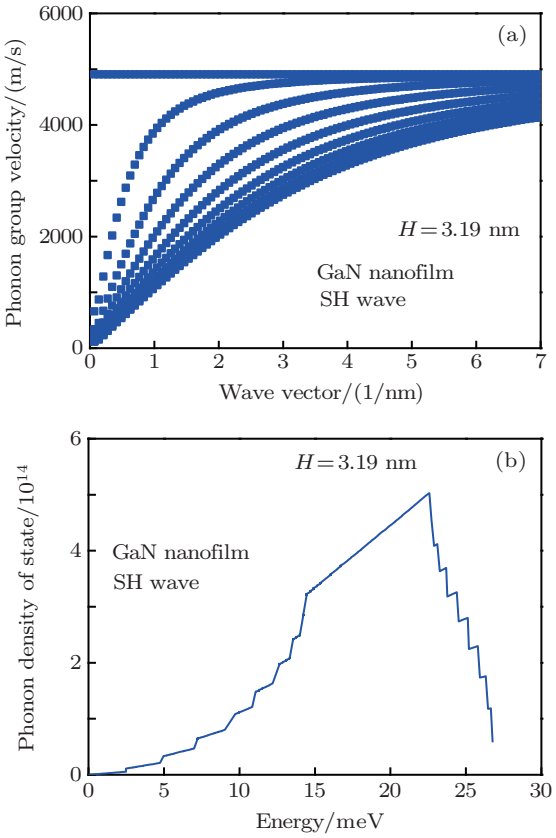


Fig. 2. (color online) Plots of phonon group velocity versus wave vector (a) and the phonon density of state versus phonon energy (b).

Once the phonon properties such as the phonon group velocity and phonon density of state are determined, the phonon thermal conductivity then can be calculated numerically for the GaN nanofilm. As is well known that the surface phonon scattering leads to the classic size effect of phonon thermal conductivity in nanostructures. We first simulate the thermal conductivity of GaN nanofilm which only suffers the surface scattering effect. Figure 3 shows the plots of the ratio of thermal conductivity versus thickness of GaN nanofilm with different values of phonon mean free path Λ and different values of specular scattering fraction p. Here, κ_0 is the bulk thermal conductivity at 300 K, and the specular scattering fraction p is 1. As shown in Fig. 3(a), with the nanofilm thickness increasing from 1000 nm to 5000 nm, the slopes for all curves of phonon thermal conductivity are very small and then the whole curves become flat. It means that the size effect of the thermal conductivity can be neglected when the film thickness is greater than several micrometers. When the film thickness falls below around 1000 nm, the thermal conductivity declines rapidly with the geometrical size of the nanofilm decreasing. Moreover, the thermal conductivity can be improved with increasing the phonon MFP. However, the influence of mean free path on the thermal conductivity becomes weaker and ultimately disappears as the film thickness is smaller than several hundred nanometers. We also show the size-dependent phonon thermal conductivities of GaN nanofilm for different values of specular scattering fraction p in Fig. 3(b). One can find that the thermal conductivity is independent of the specular scattering fraction p.

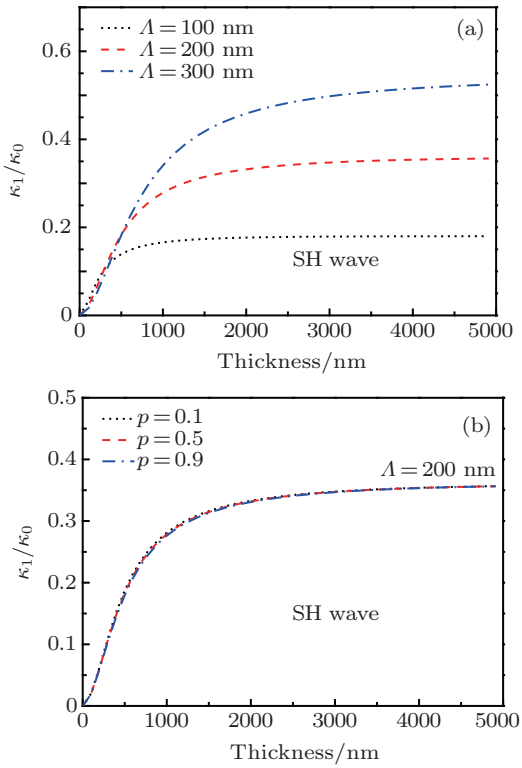


Fig. 3. (color online) Variations of phonon thermal conductivity with nanofilm thickness for different values of mean free path Λ (a) and different values of specular scattering fraction p (b).

When the nanofilm thickness varies from 1 nm to 20 nm, the surface scattering effect and quantum confinement effect must be taken into account simultaneously. Here, the size-dependent phonon thermal conductivities are calculated in the three cases, namely (i) only affected by the quantum confinement effect (QCE); (ii) only affected by the surface scattering effect (ISE); (iii) affected simultaneously by the quantum confinement effect and the surface scattering effect (QCE + ISE), as shown in Fig. 4. One can note from the figure that the phonon thermal conductivity decreases with the film thickness decreasing in all cases. With considering only the quantum confinement effect, the phonon thermal conductivity drops sharply and manifests the size effect dramatically only when

the film thickness drops to a few nanometers. While considering only the surface scattering effect, the phonon thermal conductivity reduces more rapidly with the film thickness decreasing. When the quantum confinement effect and the surface scattering effect both are considered, the surface scattering effect is more intense, leading to a two-orders-of-magnitude reduction of the thermal conductivity of GaN nanofilm compared with that of the bulk counterpart.

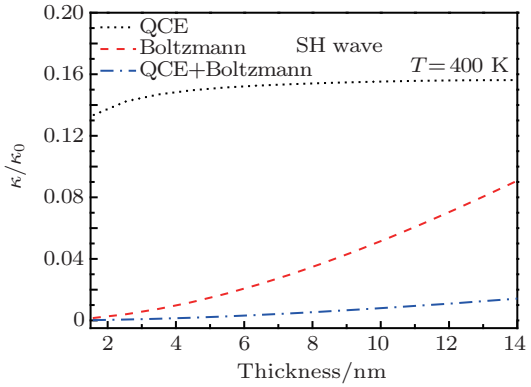


Fig. 4. (color online) Influences of the quantum confinement effect and the surface scattering effect on the phonon thermal conductivity.

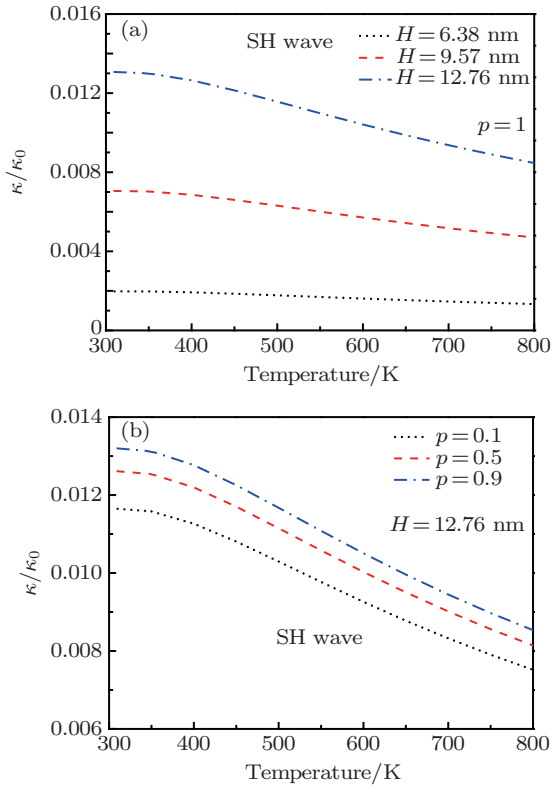


Fig. 5. (color online) Variations of phonon thermal conductivity with temperature ranging from 300 K to 800 K for (a) different geometrical sizes of the nanofilms and (b) different values of specular scattering fractions.

With comprehensively considering the quantum confinement effect and the surface scattering effect, the variations of phonon thermal conductivity with the temperature, the thickness of nanofilm and the specular scattering fraction are investigated, respectively. Figure 5 shows the temperature-dependences of phonon thermal conductivity of SH mode for different geometrical size films and different specular scattering fractions. As shown in Fig. 5, it is clearly found that the phonon thermal conductivity decreases with temperature increasing from 300 K to 800 K. From Fig. 5(a), one can note that the phonon thermal conductivity decreases with the nanofilm thickness decreasing, and the influence of the film thickness on thermal conductivity becomes smaller as temperature rises. It is also noticed from Fig. 5(b) that the thermal conductivity is enhanced with increasing the specular scattering fraction. It means that the increase in the portion of surface diffuse phonon scattering has a negative effect on the thermal conductivity of GaN nanofilm.

The variations of phonon thermal conductivity with the specular scattering fraction and geometrical size for different temperatures are shown in Figs. 6(a) and 6(b), respectively. Clearly, the gradual rise in temperature makes the thermal conductivity decrease, which corresponds to the results in Fig. 5. It follows from Fig. 6(a) that the increase of the specular scattering fraction increases the thermal conductivity. It is also noticed from Fig. 6(b) that with the geometrical size of nanofilm decreasing, the phonon thermal conductivity declines rapidly, indicating that the size effect on the phonon thermal conductivity is enhanced by the surface scattering effect.

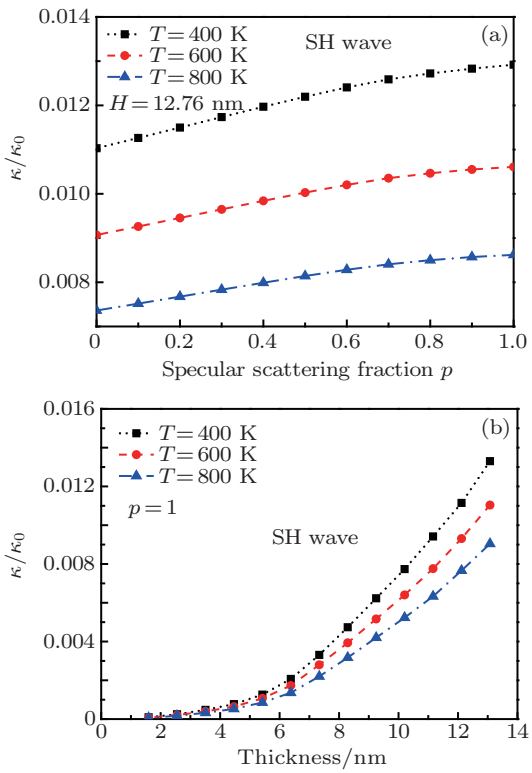


Fig. 6. (color online) Variations of phonon thermal conductivity with (a) specular scattering fractions, and (b) the geometrical size of the nanofilm for different temperatures.

Figure 7 shows the comparison between the size-dependent thermal conductivities predicted by the present model and those from some other analytical models given by Hua and Cao[56] and Majumdar.[37] In order to compare these numerical results more conveniently, the figure is plotted by

using H/Λ_0 as the horizontal axis and κ/κ_0 as the vertical axis. It is clear that the numerical results obtained by Hua *et al.* and Cao[56] agree accord well with the results from Majumdar,[37] and the thermal conductivity predicted by the present model is much smaller than the other two numerical results due to the quantum confinement effect, denoting that the quantum confinement effect manifests the size effect dramatically. Above all, it is also confirmed that the increase of nanofilm thickness increases the phonon thermal conductivity.

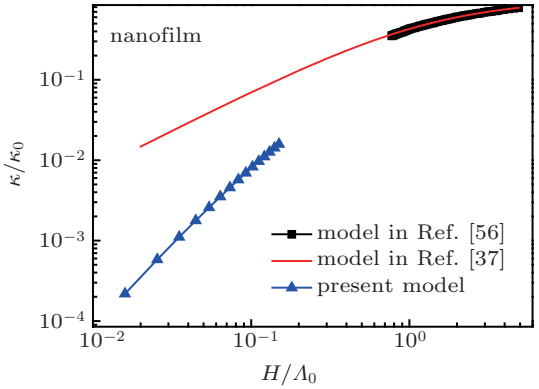


Fig. 7. (color online) Comparison of the thermal conductivities predicted by the current model and other analytical models.

4. Conclusions

In this work, the influence of the surface scattering effect on the cross-plane phonon thermal conductivity of spatially confined GaN nanofilm is investigated based on the continuum elasticity theory and the Boltzmann transport equation. Theoretical results show that when only the quantum confinement effect is taken into account, the phonon thermal conductivity can be improved by lowering the temperature or increasing the geometrical size of GaN nanostructure. While considering only the surface scattering effect, the phonon thermal conductivity can also be increased with the phonon MFP and the specular scattering fraction increasing. With comprehensively considering the two effects above, the surface scattering effect becomes enhanced dramatically with the gradual decrease of thickness of the nanofilms, resulting in two-order-of-magnitude reduction of the cross-plane thermal conductivity of nanostructures compared with that of the bulk counterpart. This work will be helpful in controlling the thermal performances in GaN nanostructures and nanoelectronic devices.

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