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ABSTRACT

Thermal performance of nanomaterials has always been a significant part of semiconductor research, which is the key problem in the development and design of various micro/nanoelectronic devices. In this work, we investigate the thermal properties of prestressed gallium nitride nanofilms based on phonon Boltzmann transport approach and acoustoelastic theory. The influence of surface/interface scattering and stress fields on phonon properties and thermal conductivity is taken into account to predict the thermal conductivity of gallium nitride nanofilms. Theoretical calculations show that the phonon surface scattering and prestress fields can modify phonon thermal conductivity of gallium nitride nanofilms significantly. The compressive stress increases thermal conductivity whilst the tensile stress decreases thermal conductivity, and phonon surface scattering decreases the conductivity of gallium nitride nanofilms. With the decrease of the structural size, the surface scattering effect is enhanced, making phonon thermal conductivity a few orders of magnitude smaller than bulk value. This work could be helpful in optimizing the phonon thermal conductivity of nanomaterials through the stress/strain engineering and the surface/interface engineering. It can also provide a piece of theoretical evidence for the design of high-performance nanodevices.

I. INTRODUCTION

Gallium nitride (GaN), as a representative of the third-generation semiconductor materials, has features of large band-gap, high breakdown electrical field, high thermal conductivity and strong radiation resistance. These characteristics make GaN especially suitable for applications in high-temperature and high-powers,[1–6] high-frequency microwave devices[7,8] and optoelectronic devices.[9–13] When the feature size of GaN-based structure is down to nanometer scale, the heat loss of device rises significantly and thermal conductivity decreases several orders of magnitude than the bulk value. Due to the direct correlation of thermal conductivity with thermal dissipation efficiency, the accurate measurement and prediction of phonon thermal conductivity could play an essential role in improving various performances of semiconductor nanodevices and designing excellent electronic power devices.

As an important property of semiconductors, phonon thermal conductivity in semiconductor nanostructure has been paid lots of attentions, including the size effect of phonon thermal conductivity and the relationship between thermal conductivity and phonon properties such as average velocity and phonon density of states (DOS). For example, Majumda[14] suggested that heat conduction induced by lattice vibration or phonon transport could be treated as heat radiation problem, and phonon thermal conductivity satisfies the black-body radiation law when the size of nanofilms is small enough. Balandin *et al.*[15,16] proposed the concept of phonon engineering to tune the thermal properties by modifying the phonon properties in semiconductor nanostructures. Szwejkowski *et al.*[17] employed time domain thermal reflection

method to analyze the size-dependent phonon thermal conductivity in β-Ga_2O_3 nanostructures. Anaya *et al.*[18] proved that thermal conductivity of nanostructures is significantly smaller than that of bulk materials in ultra-thin nanocrystalline films due to the change of grain size and contribution of the grain boundaries. Besides, researches have also focused on the optimization of the heat conductivity and heat management in nanodevices such as high electron mobility transistors (HEMTs).[19-22]

On the other hand, a great number of researches provide valuable insights into the surface and interface scattering effects on thermal properties of semiconductor nanostructures.[23-26] Since the phonon transport can be regarded as particle transport, phonon scattering on surface/interface is treated as boundary conditions in phonon Boltzmann transport equation to analyze size effect of phonon thermal conductivity. Chen[23] established a theoretical model of phonon transport and thermal conductivity based on Boltzmann transport approach, in which phonon heat flows along the thickness direction of a thin film, and analyzed the temperature distribution, boundary thermal resistance and thermal conductivity of films theoretically. Kamatagi *et al.*[24] studied thermal conductivity of wurtzite GaN from 4.2 to 400K using Holland model and modified Callaway model respectively, and described the intrinsic phonon-phonon scattering mechanism with a single set of numeric values. AlShaikhi *et al.*[25] discussed the influence of Umklapp phonon-phonon scattering on the lattice thermal conductivity of GaN bulk and nanofilms under different temperatures utilizing Callaway's relaxation-time theory. Considering the effects of phonon dispersion relation and boundary scattering during phonon transport, Zhou and Li[26] adopted Boltzmann transport equation to investigate the variation of thermal conductivity in GaN nanotubes with internal and external diameters from several nanometers to 120nm.

Owing to the GaN-based sandwich-type structures in nanoelectronic components, the lattice strain between nanometer-scale layers leads to the prestress fields and interface stress. These stress fields influences the electrical and thermal performance as well as reliability in the nanoelectronic devices.[27-30] Therefore, Liangruksa and Puri[31] studied the lattice thermal conductivity of silicon nanowires under surface stress. They found that the surface stress could decrease the lattice thermal conductivity of nanowires. Zhu *et al.*[32-35] systematically investigated the effects of external prestress and surface stress on phonon properties and phonon thermal conductivity of GaN nanofilms. It demonstrates that both prestress and surface stress change phonon properties remarkably, such as phonon dispersion relation, and eventually alter phonon thermal conductivity. Nevertheless, the influence of surface/interface scattering and prestress fields on phonon thermal conductivity has not been reported in existing literatures.

In this work, the phonon transport approach and elastic model are used to construct the theoretical model for simulation of the phonon thermal conductivity in stressed GaN nanofilms. The acoustoelastic theory is employed to calculate the phonon properties in stressed GaN nanofilms. Through solving Boltzmann transport equation, phonon surface scattering effects are considered in boundary conditions. With the aid of defining the thermal conductivity, we obtain the expression of phonon thermal conductivity in stressed GaN nanofilms, in which the influences of surface scattering and prestress fields on thermal performance are demonstrated. Numerical results demonstrate that the stress field and boundary scattering can significantly affect the phonon thermal conductivity of GaN nanofilms. Temperature- and thickness-dependent thermal conductivities are sensitive to the stress fields and boundary phonon scattering. This work could be conducive to adjusting and optimizing thermal conductivity of semiconductor nanostructures through stress/strain engineering and surface/interface engineering.

II. STRESS EFFECTS ON PHONON PROPERTIES IN GaN NANOFILMS

A. Elastic model for spatially confined phonons

Since the phonon is defined as a quantum of vibration energy which transfers to the lattice, the vibration properties of atoms are sensitive to the phonon properties. The stress fields could alter the vibration frequency of atoms, leading to the change of the phonon properties in nanostructures which could be well described by the elastic model.[15,26,32-35] A monolayer GaN nanofilm is taken as an example which is assumed to be isotropic in natural states shown in figure 1. Suppose that the phonon heat flows along the x_1 direction, and the GaN nanofilms is subjected to in-plane biaxially lateral prestresses. The initial stress field can thus be written as

$$\sigma_{11}^0 = \sigma_{22}^0 = \sigma_0, \sigma_{3i}^0 = 0. \tag{1}$$

The variable with subscript as 1 or 2 denotes the in-plane direction, whereas a subscript 3 denotes the transverse direction. The corresponding prestrains of the nanofilms can be derived as follows[32]

$$u_{11}^0 = \frac{s_{22} - s_{12}}{s_{11}s_{22} - s_{12}^2}\sigma^0, u_{22}^0 = \frac{s_{11} - s_{12}}{s_{11}s_{22} - s_{12}^2}\sigma^0, u_{33}^0 = -\frac{C_{13}}{C_{33}}u_{11}^0 - \frac{C_{23}}{C_{33}}u_{22}^0. \tag{2}$$

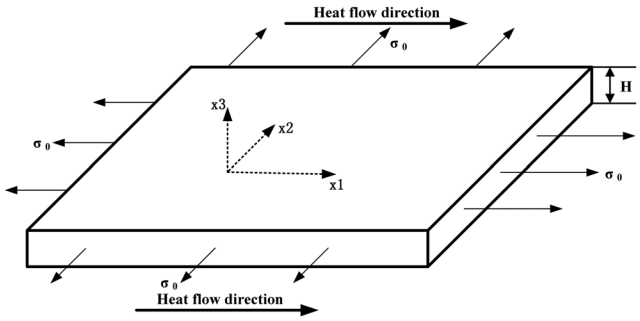

FIG. 1. Schematic drawing of GaN nanofilm under in-plane prestress field.

Here, $s_{11} = C_{11} - C_{13}^2/C_{33}, s_{12} = C_{12} - C_{13}C_{23}/C_{33}, s_{22} = C_{22} - C_{23}^2/C_{33}$. The acoustoelastic vibration equation describing the phonon in stressed nanostructure can be expressed as[36,37]

$$\rho^{new}\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j}(\bar{C}_{ijkl}\frac{\partial u_k}{\partial x_l}) + \sigma^0\frac{\partial^2 u_i}{\partial x_1^2}. \tag{3}$$

Here, $\bar{C}_{ijkl}$ represents the modified second-order elastic modulus, given by

$$\bar{C}_{ijkl} = C_{ijkl}\left(1 + u_{ii}^0 + u_{jj}^0 + u_{kk}^0 + u_{ll}^0 - u_{11}^0 - u_{22}^0 - u_{33}^0\right) + C_{ijklmn}u_{mn}^0. \tag{4}$$

Non-zero components of the effective modulus can be expressed as

$$\begin{aligned}
\bar{C}_{11} &= \bar{C}_{22} = C_{11}\left(1 + 2u_{11}^0 - u_{33}^0\right) + (C_{111} + C_{112})u_{11}^0 + C_{112}u_{33}^0\\
\bar{C}_{33} &= C_{11}\left(1 + 2u_{11}^0 - u_{33}^0\right) + 2C_{112}u_{11}^0 + C_{111}u_{33}^0\\
\bar{C}_{13} &= \bar{C}_{23} = C_{12}(1 + u_{33}^0) + (C_{123} + C_{112})u_{11}^0 + C_{112}u_{33}^0\\
\bar{C}_{12} &= C_{12}(1 + u_{33}^0) + 2C_{112}u_{11}^0 + C_{123}u_{33}^0\\
\bar{C}_{44} &= \bar{C}_{55} = C_{44}(1 + u_{33}^0) + (C_{144} + c_{155})u_{11}^0 + C_{155}u_{33}^0,
\end{aligned} \tag{5}$$

and $\bar{C}_{66} = (\bar{C}_{11} - \bar{C}_{12})/2$. ρ^{new} is the density of GaN nanofilms after deformation. When heat flow propagates along the direction of x_1 as shown in figure 1, the displacements of the nanofilms are the functions of x_1 and x_3. One can write the solution of vibration equation as follows,

$$\mathbf{u} = \hat{\mathbf{u}}(x_3)\exp[i(\omega t - q_0 \cdot x_1)], \tag{6}$$

where ω is phonon frequency, and q_0 is wave vector. $\hat{\mathbf{u}}$ is defined as the amplitude of displacement vector. Substituting the equation (6) into the vibration equation (3), one can and obtain

$$\begin{bmatrix}
\bar{C}_{44}\frac{d^2}{dx_3^2} - (\bar{C}_{11} + \sigma^0){q_0}^2 & 0 & -iq_0(\bar{C}_{13} + \bar{C}_{44})\frac{d}{dx_3}\\
0 & \bar{C}_{44}\frac{\partial^2}{\partial x_3^2} - (\bar{C}_{66} + \sigma^0){q_0}^2 & 0\\
-iq_0(\bar{C}_{13} + \bar{C}_{44})\frac{d}{dx_3} & 0 & \bar{C}_{33}\frac{d^2}{dx_3^2} - (\bar{C}_{44} + \sigma^0){q_0}^2
\end{bmatrix}\hat{\mathbf{u}}(x_3) = -\rho^{new}\omega^2\hat{\mathbf{u}}(x_3), \tag{7}$$

According to classical elastic vibration theory,[38] there are three modes of phonons in films. That is, shear mode (SH), dilatational mode (SA) and flexural mode (SA). For SH mode,

$$u_2 = \hat{u}_2(x_3)\exp[i(\omega t - q_0 \cdot x_1)]. \tag{8}$$

Substituting u_2 into Eq. (7), we have

$$\bar{C}_{44}\frac{d^2\hat{u}_2}{dx_3^2} + \left[\rho^{new}\omega^2 - (\bar{C}_{66} + \sigma^0)q_0^2\right]\hat{u}_2 = 0. \tag{9}$$

For SA and AS modes, $\mathbf{u} = (u_1, 0, u_3)$. Thus, we can obtain

$$\begin{cases}
\bar{C}_{44}\frac{d^2\hat{u}_1}{dx_3^2} - iq_0(\bar{C}_{13} + \bar{C}_{44})\frac{d\hat{u}_3}{dx_3} + \left[\rho^{new}\omega^2 - (\bar{C}_{11} + \sigma^0)q_0^2\right]\hat{u}_1 = 0\\
\bar{C}_{33}\frac{d^2\hat{u}_3}{dx_3^2} - iq_0(\bar{C}_{13} + \bar{C}_{44})\frac{d\hat{u}_1}{dx_3} + \left[\rho^{new}\omega^2 - (\bar{C}_{44} + \sigma^0)q_0^2\right]\hat{u}_3 = 0.
\end{cases} \tag{10}$$

When the top and bottom surfaces of the nanofilms are free, the boundary conditions can be expressed as

$$\sigma_{23} = \frac{\partial u_2}{\partial x_3} = 0 \tag{11a}$$

$$\sigma_{13} = \frac{\partial u_1}{\partial x_3} - iq_0u_3 = 0, \sigma_{33} = \bar{C}_{33}\frac{\partial u_3}{\partial x_3} - iq_0\bar{C}_{13}u_1 = 0. \tag{11b}$$

Here, Eq. (11a) is the boundary condition for SH mode, while Eq. (11b) is the boundary condition for SA and AS modes. Combining Eqs. (9)–(11), the dispersion relations of different modes can be calculated using the finite difference method.

B. Phonon properties of stressed GaN nanofilms

Once the phonon dispersion relations of different modes in nanofilms are derived, the phonon frequency varied with the phonon wave vector q can be calculated using the finite difference method. Thus, the phonon group velocity of various modes can be determined by a numerical differentiation, given by

$$v_n(q_0) = d\omega_n(q_0)/dq_0, \tag{12}$$

in which the subscript n is the number of phonon branches. The average phonon group velocity $\bar{V}(\omega)$ is used to character the velocity of wave package with every mode populated for each polarization, which can be defined as[32]

$$\bar{V}(\omega) = \left\{\frac{1}{m(\omega)}\sum_{n=1}^{m(\omega)}[v_n(\omega)]^{-1}\right\}^{-1}, \tag{13}$$

The thermal properties of semiconductors are not only relevant to the phonon group velocity, but also related to the phonon density of states (DOS). One can combine the group velocity and confined phonon dispersion relations to obtain the quasi-2D phonon DOS in GaN nanofilms, given as

$$f_n^{SA,AS,SH}(\omega) = \frac{1}{H}\left[\frac{1}{2\pi}q_{0n}^{SA,AS,SH}(\omega)\frac{1}{v_n^{SA,AS,SH}}\right], \tag{14}$$

Hence, the total phonon density of state can be reached for all polarizations by summing up n phonon branches as $F(\omega) = \sum_n f_n(\omega)$.

III. PHONON SURFACE SCATTERING EFFECTS ON PHONON TRANSPORT

A. Phonon Boltzmann transport approach

Boltzmann transport approach is a general and powerful method for study of the energy transport phenomenon in nanostructures. Here, we use the phonon Boltzmann equation under the approximation of relaxation time to derive the phonon thermal conductivity in stressed GaN nanofilms. Phonon energy strength I can be defined as[14,23]

$$I = \frac{1}{4\pi}\sum_m \int_0^{\upsilon_{\max}} |v_m| f h v D_m(v) dv. \tag{15}$$

Here, v_m refers to the amplitude of phonon group velocity. f is the function of phonon distribution, while h is Planck constant. ω is phonon frequency, and D is the density of states of phonons in a unit volume. For GaN nanofilms, when heat propagates along the direction of x_1, the phonon transport inside the GaN naonfilm can be described by phonon Boltzmann transport equation, that is

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

Therein, I_0 is the phonon energy strength in the equilibrium state. Phonon distribution function f satisfies Bose-Einstein distribution function. θ and φ refers to the polar angle (solid angle) and azimuth angle, respectively. $\Lambda = |\mathbf{v}|\tau$ is the phonon mean free path. Here, τ is the phonon relaxation time, following the Matthiessen's rule, $\tau_T^{-1} = \tau_U^{-1} + \tau_M^{-1} + \tau_{ph-e}^{-1}$, where τ_U is the Umklapp scattering rate, τ_M is the point-defect scattering rate, τ_{ph-e} is the electron-acoustic phonon scattering rate.

Due to the phonon surface scattering in the nanofilms, the phonon distribution function f will be only related to x_3. It means that phonon strength I is uniform in the in-plane along the direction of x_1 and x_2, while it varies with x_3 along the thickness direction of the film. Introducing the deviation function $i(x_3,\theta) = I(x_3,\theta) - I_0(T)$ and substituting it into Eq. (16), we obtain

$$\sin\theta\sin\varphi\frac{\partial i}{\partial x_3} + \frac{i}{\Lambda} = -\sin\theta\sin\varphi\frac{dI_0}{dx_3} \quad (0 < \theta < \pi, 0 < \varphi < 2\pi). \tag{17}$$

Through solving differential Eq. (17), one can get the solution of the deviation function i. That is, in the case of $0 < \theta < \pi/2$,

$$i(\eta,\mu) = i^+(\eta,\mu) = \begin{cases} i^+(0,\mu)e^{-\eta/\mu} - \int_0^\eta \frac{dI_0}{dt}e^{-(\eta-t)/\mu}dt & (0<\mu<1, 0<\varphi<\pi) \\ i^+(\xi,\mu)e^{(\xi-\eta)/\mu} + \int_\eta^\xi \frac{dI_0}{dt}e^{-(\eta-t)/\mu}dt & (-1<\mu<0, \pi<\varphi<2\pi), \end{cases} \tag{18}$$

and in the case of $\pi/2 < \theta < \pi$,

$$i(\eta,\mu) = i^-(\eta,\mu) = \begin{cases} i^-(0,\mu)e^{-\eta/\mu} - \int_0^\eta \frac{dI_0}{dt}e^{-(\eta-t)/\mu}dt & (0<\mu<1, 0<\varphi<\pi) \\ i^-(\xi,\mu)e^{(\xi-\eta)/\mu} + \int_\eta^\xi \frac{dI_0}{dt}e^{-(\eta-t)/\mu}dt & (-1<\mu<0, \pi<\varphi<2\pi). \end{cases} \tag{19}$$

Here, $\mu = \sin\theta\sin\varphi$, $\eta = x_3/\Lambda$ and $\xi = H/\Lambda$. H is the thickness of the GaN nanofilms.

To determine the coefficients in $i^+(\eta,\mu)$ and $i^-(\eta,\mu)$, boundary conditions of phonon surface/interface scattering are needed. There are several modes of surface/interface scattering, which are generally divided into full diffuse scattering model, full specular scattering model, and partial diffuse partial specular model.[39] Here, we adopt the partial diffuse-partial specular scattering model, and assume that the surface/interface specular scattering coefficient p indicates the proportion of specular scattering in total. When heat transfers along the direction of x_1, the sketch maps of surface/interface scattering are shown in figure 2.

When phonons are incident on the surface of nanofilms, two kinds of interface scatterings will occur simultaneously. For a monolayer nanofilms, energy transmissivity R is considered while energy transmissivity T is neglected. For distinguishing, R_s denotes the energy transmissivity of specular scattering and R_d represents the energy transmissivity of diffuse scattering. Following the energy conservation law and symmetry conditions, phonon energy balance equation on the upper surface is given as

$$I^+(\xi, -\mu) + I^-(\xi, -\mu) = pR_s(\mu)[I^+(\xi,\mu) + I^-(\xi,\mu)] + \frac{2(1-p)}{\pi}R_d \times \int_0^\pi \left[\int_0^1 (I^+(\xi,\mu) + I^-(\xi,\mu))\alpha d\alpha\right] d\varphi, \tag{20}$$

and phonon energy balance equation on the lower surface is given as

$$I^-(0,\mu) + I^+(0,\mu) = pR_s(\mu)[I^-(0, -\mu) + I^+(0, -\mu)] + \frac{2(1-p)}{\pi}R_d \times \int_\pi^{2\pi} \left[\int_0^1 (I^-(0, -\mu) + I^+(0, -\mu))\alpha d\alpha\right] d\varphi. \tag{21}$$

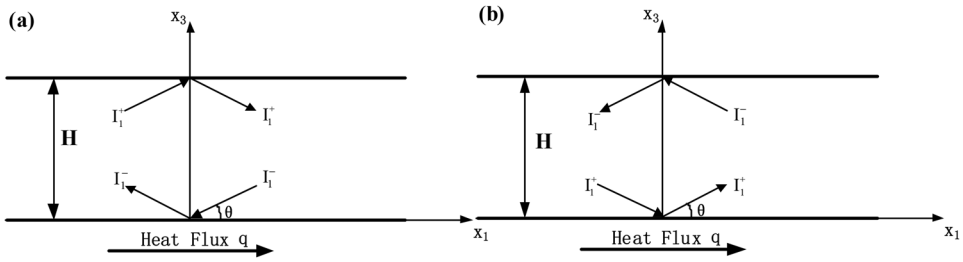

FIG. 2. Schematic drawing of phonon surface scattering during heat transport.

From the Eqs. (20) and (21), the corresponding $i^+(0,\mu)$ and $i^-(\xi,\mu)$ can be derived. The heat flow q along the x_1 direction can be obtained eventually on the basis of definition of phonon heat flow:

$$q(\eta) = \int_{4\pi} \mathrm{I}\cos\theta d\Omega = \int_0^{\pi}\left[\int_0^1 (i^+(\eta,\mu) - i^+(\eta,-\mu) + i^-(\eta,\mu) - i^-(\eta,-\mu))\alpha d\alpha\right]d\varphi. \quad (22)$$

Here, Ω is the differential stereoscopic angle, and $d\Omega = \sin\theta d\theta d\varphi$.

B. Phonon thermal conductivity of GaN nanofilms

Since phonon heat flows along the direction of x_1, in-planar phonon thermal conductivity κ can be derived by Fourier' law[40]

$$q = -\kappa\nabla \mathrm{T}, \quad (23)$$

where ∇T refers to temperature gradient. If the phonon thermal conductivity involved spatial confinement effects is marked as κ_1, the thermal conductivity simultaneously affected by spatial confinement and surface/interface scattering can be marked as κ, then one can get

$$\kappa = \kappa_1 \mathrm{G}_0. \quad (24)$$

Here, G_0 is size-dependent function in which the surface/interface scattering effects are involved. The thermal conductive κ_1 can be expressed as below.[41]

$$\kappa_1 = \frac{1}{3}\left(\frac{k_B}{\hbar}\right)k_B \mathrm{T}\int_{x_{\min}}^{x_{\max}} \frac{x^2 e^x}{(e^x-1)^2}\tau(x)\bar{\mathrm{V}}^2(x)\mathrm{F}(x)dx = \kappa_0 \mathrm{G}_1, \quad (25)$$

in which $\hbar = h/2\pi$, and $x = \hbar\omega_n(\mathbf{q})/k_B\mathrm{T}$. $\bar{\mathrm{V}}$ refers to phonon average group velocity, and F indicates the total density of states of phonon, κ_0 represents the bulk phonon thermal conductivity of GaN. G_1 is the function describing the spatial confinement effect on conductivity. Thereby, the phonon thermal conductivity of stressed GaN films can be rewritten as

$$\kappa = \kappa_0 \mathrm{G}. \quad (26)$$

Here, $\mathrm{G} = \mathrm{G}_0\mathrm{G}_1$ represents the function to character the influence of the spatial confinement, stress fields and phonon surface scattering.

IV. RESULTS AND DISCUSSION

To explore the influence of surface/interface scattering and prestress field on the phonon thermal conductivity of GaN nanofilms, we take SH mode of wurtzite GaN as an example here to carry out numerical calculations. Elastic moduli of bulk GaN are as follows, C_{33} = 252GPa, C_{13} = 129GPa,C_{44} = 148GPa. Other physical parameters are choosen from literatures.[42–45]

Firstly, the phonon properties for SH mode such as dispersion relations, phonon group velocity and density of states in stressed GaN nanofilms are simulated. Figure 3a shows the phonon energy varied with wave vector under different prestress fields, in which phonon wave vector q_0 varies from 0 to π/a, a is the lattice constant. It is clearly shown that the negative stress increases the slope of various phonon dispersion modes, whereas the positive stress reduces it. In other words, negative stress increases phonon energy whilst positive stress decreases it. Figure 3b illustrates the variation of phonon average group velocity with phonon energy under different prestresses. Apparently, phonon average group velocity is equal to phonon group velocity at low-energy region. Along with the increases of phonon energy, the group velocity starts to oscillate continuously. This is because the phonon average velocity is the superposition of varies modes, and it oscillates at the intersection point of each modes. Besides, negative stress increases the velocity but positive stress reduces the velocity. Figure 3c depicts the variation of phonon density of states with the phonon energy of nanofilms under different prestresses. Similarly, phonon density of states increase with phonon energy in a step-up way and reach the peak, then decline subsequently. Negative stress decreases the density while positive stress improves the velocity.

Then, phonon surface scattering effects on in-plane thermal conductivity of GaN nanofilms are analyzed by solving Eqs. (19)–(21). Figure 4 shows the variation of phonon thermal conductivity with thickness of GaN nanofilms under different phonon mean free path. Here, κ_0 indicates phonon thermal conductivity of bulk GaN at 300K. As figure 10(a) shown, thermal conductivity increases slowly with the thickening of nanofilms and the curve tends to be horizontal when the thickness is greater than several micrometers. It demonstrates that size effect can be neglected when film thickness is large enough. While the structure size drops to several hundreds of nanometers, thermal conductivity declines rapidly with the decrease of film thickness and manifests a significant size effect. Furthermore, thermal conductivity increases with

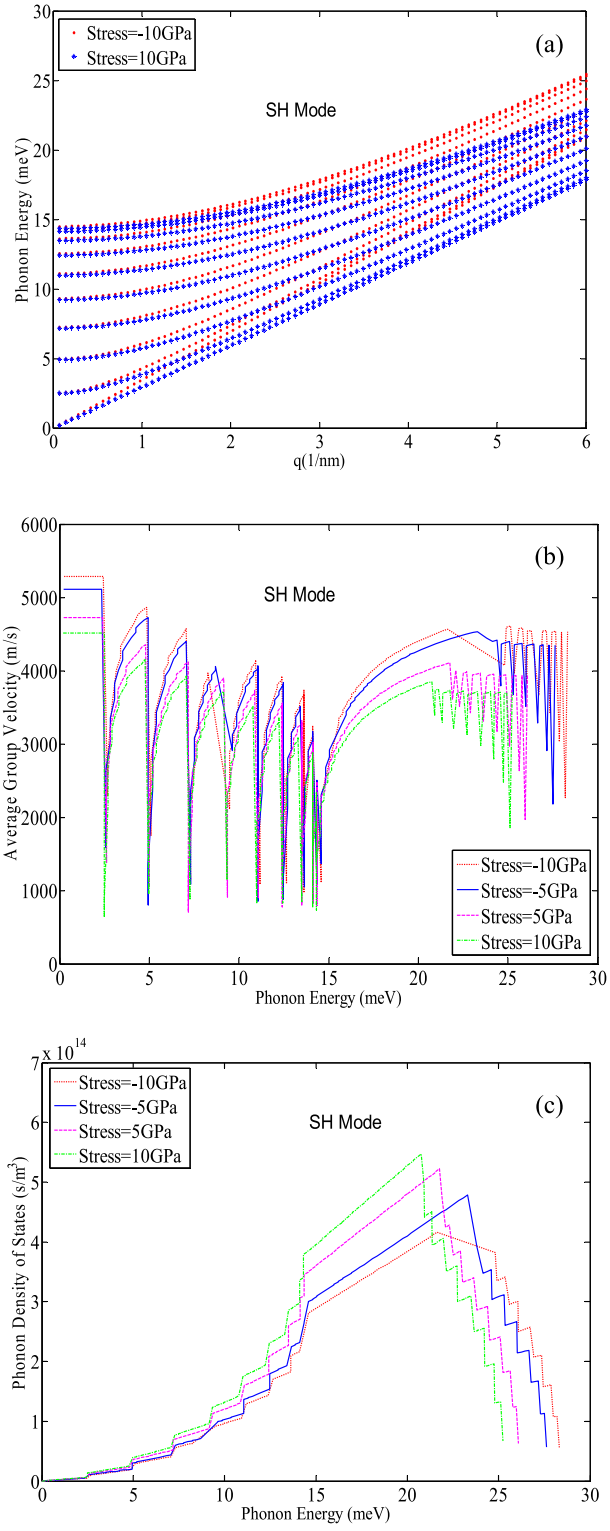

FIG. 3. Phonon energy varied with wave vector (a), phonon average group velocity (b) and phonon density of states (c) varied with energy under different prestress fields.

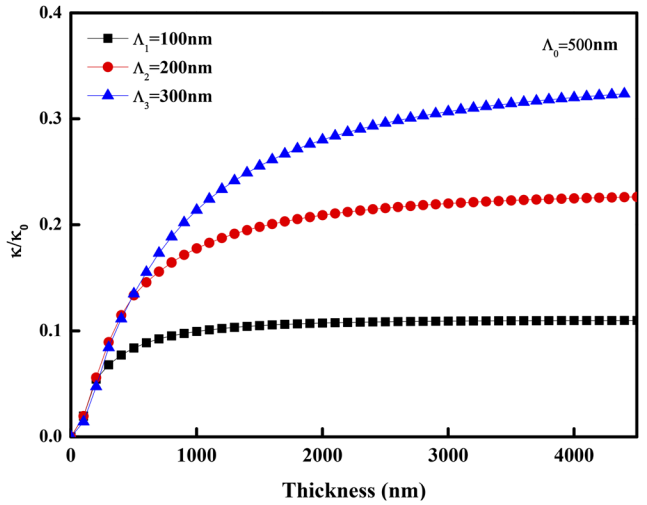

FIG. 4. Phonon thermal conductivity as a function of thickness of GaN nanofilm under different phonon mean free path Λ.

increasing the phonon mean free path Λ. While, the influence of phonon mean free path on thermal conductivity diminishes with the reduction of film thickness.

When the in-plane phonon thermal conductivity of GaN nanofilms is suffered from the spatial confinement effects and surface scattering effects, we consider three cases: (i) spatial confinement effects only (QCE), (ii) surface scattering effects only (ISE), and (iii) spatial confinement effects and surface scattering effects simultaneously (QCE +ISE). Figure 5 shows the thermal conductivity varied with the thickness under all cases above. It can be found from the figure that, for only spatial confinement effects considered, thermal conductivity declines rapidly when the thickness drops to several nanometers, showing a significant spatial size effects. For only

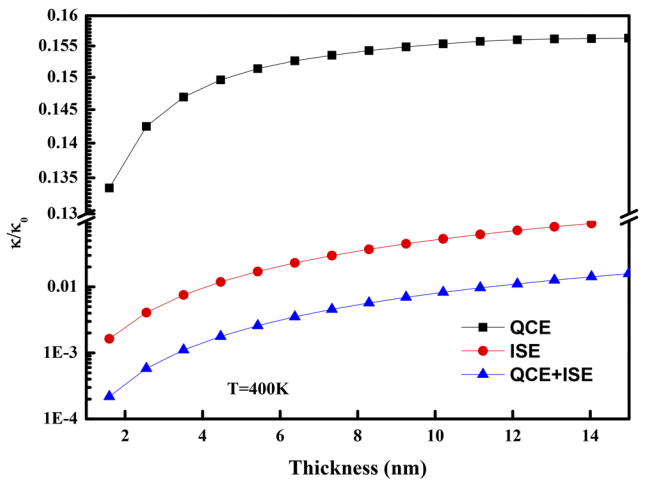

FIG. 5. Contribution of spatial confinement and surface scattering on phonon thermal conductivity of GaN nanofilms.

surface scattering effects considered, thermal conductivity performs size effects more significantly. When two effects are considered simultaneously, the surface scattering will be enhanced with the decrease of thickness, and the phonon thermal conductivity of nanofilms declines two orders of magnitude compared with bulk material.

After that, we further study the changes of phonon thermal conductivity with temperature, thickness and specular scattering coefficient considering spatial confinement and surface scattering effects comprehensively. Figure 6 shows the variation of phonon thermal conductivity with temperature under different thickness and specular scattering coefficient. Obviously, phonon thermal conductivity decreases as temperature rises as shown in figure 6. With decreasing the film thickness, thermal conductivity is reduced, which can be obtained in figure 6(a). When temperature rises, the influence of thickness on phonon thermal conductivity will be weakened. From figure 6(b), we obtain that the increase of specular scattering coefficient enhances phonon thermal conductivity. It also indicates that specular scattering has an enhancement effect on phonon thermal conductivity, and the impact of specular scattering coefficient is slightly weakened with the increase of temperature.

Figure 7 shows that phonon thermal conductivity varies with the specular scattering and thickness at different temperatures. Apparently, phonon thermal conductivity descends as temperature rises, which is identical with the results in figure 6. In figure 7(a), one can find that increasing specular scattering coefficient promotes phonon thermal conductivity. And phonon thermal conductivity declines rapidly due to the decrease of film thickness, shown in figure 7(b). The results manifest that the size effect of phonon thermal conductivity

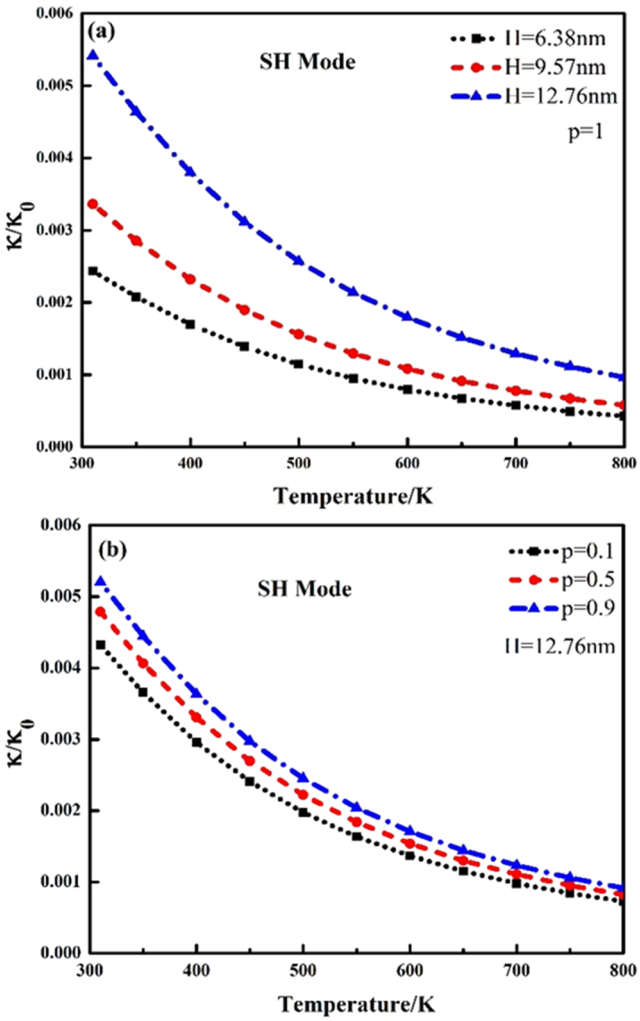

FIG. 6. Phonon thermal conductivity of GaN nanofilms as a function of temperature with different thickness (a) and different specular scattering coefficient (b).

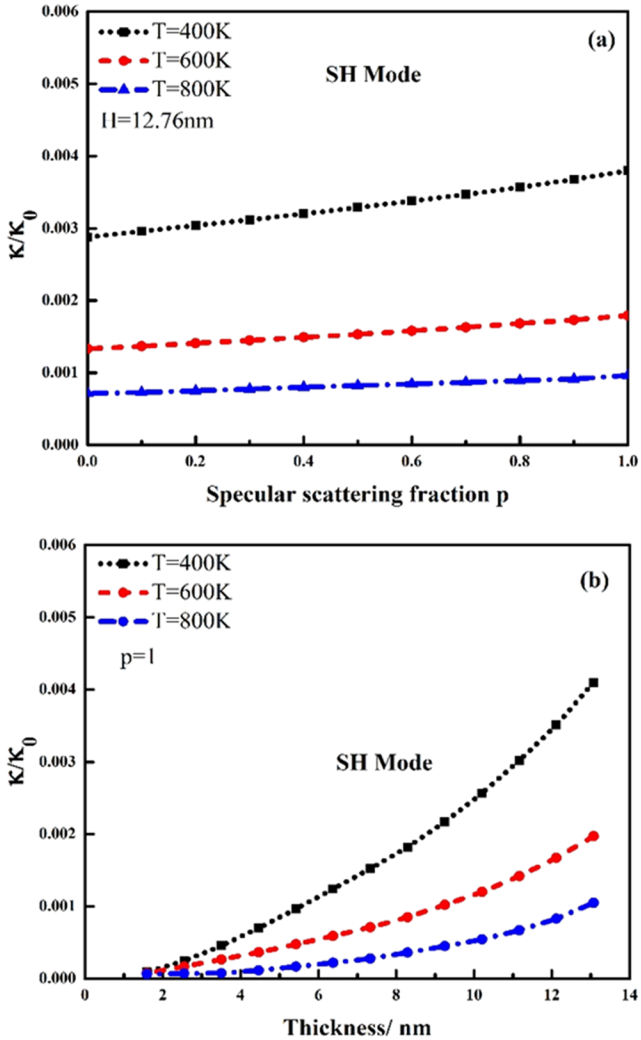

FIG. 7. Variation of phonon thermal conductivity of GaN nanofilms with specular scattering coefficient (a) and thickness (b) under different temperatures.

is notably enhanced by surface scattering effects, which coincides with the results in figure 6(b). From figures 6 and 7, it can be noted that a significant variation occurs in phonon thermal conductivity after introducing surface scattering effects and spatial confinement effects. The phonon thermal conductivity appears a reduction of two orders of magnitude and turns to be one percent of bulk value.

Finally, we studied the impact of surface scattering effect and spatial confinement effect on phonon thermal conductivity of GaN nanofilms under prestress fields. Figure 8 plots the variation of phonon thermal conductivity with temperature under different prestresses in GaN nanofilms. Obviously, phonon thermal conductivity rises along with the increase of temperature in the range of 0 to 800K. Thermal conductivity reaches peak value at 200 to 250K, and declines rapidly in pace with the increase of temperature. It can also be noticed from the figure that with the increase of the stress from -10 GPa to 10 GPa, phonon thermal conductivity increases in low temperature region, whereas it is decreased in high temperature region. Furthermore, the influence of prestress on κ is gradually weakened as temperature rises after 200 T.

Figure 9 shows the variation of the phonon thermal conductivity with the thickness of nanofilms under different prestress fields. As seen in figure 9, the phonon thermal conductivity of GaN nanofilms declines with the decrease of the thickness, and it performs significant size effect. At room temperature, compressive stress enhances thermal conductivity and tensile stress reduces thermal conductivity, comparing with the conductivity of GaN nanofilms without prestress. Figure 10 further shows the variation of phonon thermal conductivity with prestress fields under different thicknesses of GaN nanofilms. One can find that phonon thermal conductivity increases when the applied stress changes from tensile stress to compressive stress. That is, tensile stress reduces conductivity and compressive stress increases conductivity. Furthermore, the impact of compressive stress on κ is more notable than which of tensile stress. Size effect of conductivity abates rapidly with the increase of tensile stress. On the contrary, when compressive stress increases, the size effect of conductivity is enhanced.

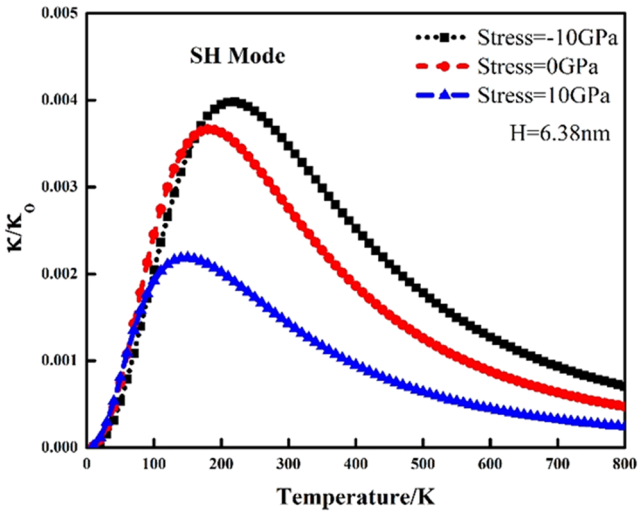

FIG. 8. Phonon thermal conductivity of GaN nanofilms as a function of temperature with different prestress fields.

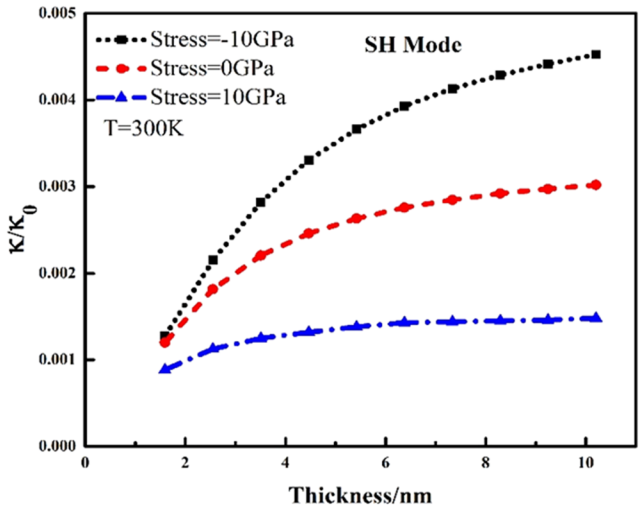

FIG. 9. Phonon thermal conductivity of GaN nanofilms as a function of thickness with different prestress fields.

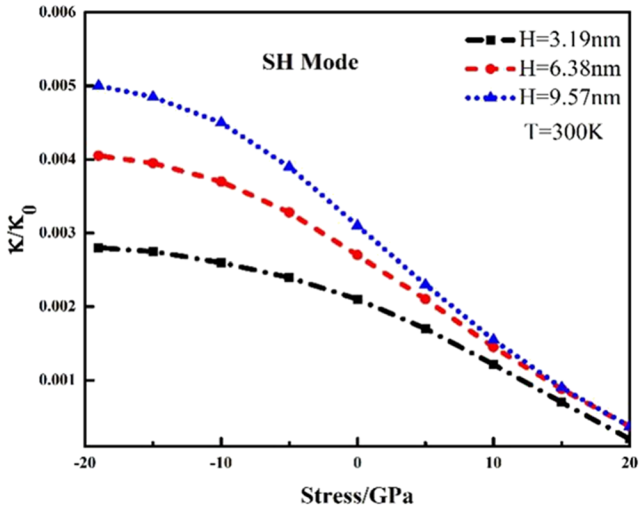

FIG. 10. Phonon thermal conductivity of GaN nanofilms as a function of prestress with different thickness.

V. CONCLUSION

In this work, we theoretically discussed the influence of spatial confinement, interface scattering and stress fields on

phonon thermal conductivity of GaN nanofilms. The acoustoelastic theory and Boltzmann transport approach are employed to derive the phonon properties and phonon thermal conductivity of stressed GaN nanofilms. The numerical results show that the phonon thermal conductivity can be increased by either decreasing the temperature, increasing the thickness of GaN film or reducing the prestress. In addition, considering surface scattering effects, the present results also show that the thermal conductivity can be significantly reduced and can be enhanced by increasing the specular scattering coefficient. As the structure size decreases, surface scattering effects could be greatly strengthened. The size-dependent phonon thermal conductivity appears a reduction of several orders of magnitude compared to that of bulk material, and it turns to be one percent of bulk value. After introducing the prestress fields, we find that positive stress decreases the thermal conductivity whereas negative stress increases it. It indicates the possibility of modifying phonon thermal conductivity through adjusting the value and direction of prestress fields. This work contributes to the optimization of phonon thermal conductivity in nanostructures based on stress/strain engineering and surface/interface scattering engineering, which would be helpful to develop proper guidelines in designing nanodevices with excellent performance.

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