Ballistic–diffusive phonon transport and size induced anisotropy of thermal conductivity of silicon nanofilms

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HIGHLIGHTS

- We establish a ballistic–diffusive model for the phonon transport in nanofilms.
- We predict the cross plane thermal conductivity of silicon nanofilms.
- We analyze the size-induced anisotropy of thermal conductivity of silicon nanofilms.

GRAPHICAL ABSTRACT
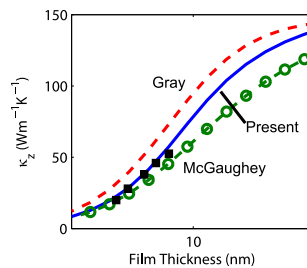
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ABSTRACT

The effective thermal conductivity of nanofilms is size dependent due to the diffusive–ballistic transport of phonons. In this paper, we investigate the cross-plane phonon transport from the viewpoint of the phonon Boltzmann equation. A predictive model for the size dependent thermal conductivity is proposed and agrees well with the results of molecular dynamics simulation for silicon nanofilms. The ballistic transport has different effects on the heat conduction in the in-plane or cross-plane directions, which causes the anisotropy of thermal conductivity of nanofilms. Such anisotropy is also size dependent and vanishes with the increase of film thickness.

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1. Introduction

In classical theory, the heat conduction obeys the Fourier's law, i.e. $q = -\kappa \nabla T$. It means that the heat flux density, q, is proportional to the temperature gradient ∇T. The coefficient, κ, is the thermal conductivity. If the material is ideally isotropic, κ is the same in all directions. The asymmetry of material will cause an anisotropic κ. For example, κ changes along different axes of a crystal; it can vary several hundred times for graphite when measured along the

plane or perpendicular to the plane. On the other hand, for layered composites, the in plane conductivity is in general different from the cross plane one because the former is determined by the sum of conductances of each layer while the latter is by the sum of resistances.

The above two cases indicate that the anisotropy of κ can either rise from the asymmetry of atomistic level (the spatial distribution of atoms in unit cell) or macroscopic level (the spatial distribution of component materials). However, in both cases κ is a constant property of the material regardless of the system size. In recent years, it has been found that the effective κ of nanostructured materials is size dependent and significantly different with their bulk counterparts [1–8]. It is recognized that Fourier's law is

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applicable in the diffusive limit, where the heat carriers are fully scattered or relaxed. In nanosystems, the heat conduction is not purely diffusive but contains a ballistic part, since the system size is comparable with the mean free path of heat carriers. Models different from Fourier's law should be used to describe the ballistic–diffusive transport, which is nonlocal and geometry sensitive. When the angle between the temperature drop direction and the characteristic size of system changes, e.g. in the in-plane or cross-plane direction of a nanofilm, the apparent thermal conductivity also changes. In this way, the effective k of nanosystems are expected to be anisotropic. Compared with previous cases, such anisotropy rises from the asymmetry of the mesoscopic level and depends on the system size. The anisotropy of κ in nanosystems is worth investigating in the light of increasing importance of energy transport in nanoscale.

To model the anisotropy of κ in asymmetric nanosystems, the ballistic–diffusive phonon transport needs to be characterized. The phonon Boltzmann transport equation (BTE) is widely used to calculate the thermal transport property of nanostructured materials. Chen [9,10] studied the cross plane transport of GaAs/AlAs and Si/Ge superlattices through the numerical solution of a single-mode relaxation-time BTE and concluded that the interface scattering significantly reduced the total κ of superlattices. The similar algorithm was applied to calculate the phonon transport in periodic two-dimensional Si/Ge nanocomposites [11], superlattice nanowires [12] and polycrystalline materials with randomly oriented superlattice grains [13]. Strong size effects of the effective thermal conductivity are observed in these systems. Maldovan [14] studied the ballistic–diffusive phonon transport in nanosystems through the Boltzmann transport equation. He found that the principle for ballistic transport should be modified by considering the combined effects of length scale, temperature, and boundary roughness. The Monte Carlo (MC) method is another powerful tool to numerically solve the BTE for nanosystems. The transport in nanowires and nanofilms was investigated in terms of the MC method and the effect of size and boundary roughness was demonstrated [15,16].

Macroscopic models based on the solution of BTE have been proposed in the past decades. These models can retain the agreement with experiments for nanosystems while avoiding heavy numerical work. Majumdar [17] formulated the equation of phonon radiative transfer (EPRT) to solve the BTE. A simple theoretical model for the effective thermal conductivity of diamond films was proposed in analogy with the photon radiative heat transfer and agrees well with the EPRT solution. Since the phonon mean free path is assumed to be independent of the phonon frequency and branch, this model was called the Gray model. McGaughey et al. [18] accounted the frequency dependent group velocity and phonon lifetimes and obtained an analytical model for the effective conductivity of nanofilms. The phonon hydrodynamics model [19–25] is proposed based on the eigenvalue solution of the linearized phonon BTE. It contains a Laplacian term of heat flux, which is similar to the viscous term in Navier–Stokes equation. Therefore, a Poiseuille flow of phonons is likely to form in small systems. The thermomass theory [26–34] establishes generalized thermal transport equations based on the momentum balance equation of phonon gas, which is consistent with the solution of phonon BTE. It is similar to the phonon hydrodynamic model with the parameters in constitutive equations having more fluidic meaning such as the phonon gas viscosity. The in-plane phonon transport in the nanofilms and nanowires was modeled by a rarefied phonon gas flow in porous medium with a size dependent viscosity and a good agreement with experiments was obtained [33,34]. In this paper, we will discuss the cross-plane κ of the Si nanofilm from the viewpoint of phonon BTE. The ballistic–diffusive phonon transport and its induced anisotropy of κ are investigated.

2. Phonon gas model and in-plane heat conduction

In dielectric solids the phonon is the main carrier of thermal energy. The thermal conductivity, κ, of a condensed matter is expressed in a similar way to that of gas [35]

$$\kappa = \tfrac{1}{3}\rho C_V v_s^2 \tau_R = \tfrac{1}{3}\rho C_V v_s \lambda_R, \tag{1}$$

where ρ is the material density, C_V is the specific heat, v_s is the mean phonon group velocity, τ_R is the average relaxation time of the resistive (R) scattering processes, $\lambda_R = v_s \tau_R$ is the corresponding mean free path. Eq. (1) is called the kinetic model which does not include the boundary effect on thermal conduction [16]. Based on the eigenvalue solution of the linearized phonon BTE, Guyer and Krumhansl [19–20] established a generalized thermal transport equation, called the GK model

$$\tau_R \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -\kappa \nabla T + l_G^2 (\nabla^2 \mathbf{q} + 2\nabla\nabla\mathbf{q}), \tag{2}$$

where l_G is a characteristic length which contains the effects of both R and normal (N) processes

$$l_G = \sqrt{\frac{\lambda_R \lambda_N}{5}}, \tag{3}$$

where $\lambda_N = v_s \tau_N$ is the mean free path of the N processes. Based on Eq. (2), the collective behavior of phonons is analogous to a fluid flow, since the Laplacian term on the right hand side is similar to the viscous dissipation term in the Navier–Stokes equation.

For the steady in-plane heat conduction in a film with a thickness H, the GK model can be simplified as [19,20]

$$-\kappa \nabla T = \mathbf{q} - l_G^2 \nabla^2 \mathbf{q}. \tag{4}$$

The left hand side of Eq. (4) is the driving term. The second term on the right hand side of Eq. (4) allows the boundary to impede the heat flow. When the system size shrinks, the boundary resistance becomes important and reduces the effective κ. If one assumes the heat flux vanishes at the boundary (non-slip) and l_G is a constant, a quadratic dependence on size of the effective κ is predicted by Eq. (4) [21–23]. However, the experimental results show a linear dependence of κ on size [2–5,21]. Given that the phonon gas is possible to exhibit rarefaction effect at high Knudsen number (Kn) cases, the assumption of non-slip boundary and constant viscosity needs to be modified. Alvarez, Jou, and Sellitto [21–23] proposed a Maxwell slip boundary condition, $q_w \propto \lambda_R \partial q / \partial r$, to replace the non-slip boundary condition and the linear size dependence was recovered. Ma [24] indicated that the non-dimensional boundary slip heat flux is proportional to the effective mean free path, which is a function of the Knudsen number. Then the effective κ of both nanofilms and nanowires are analytically derived.

In a previous work, a macroscopic phonon gas model is developed based on the thermomass theory [33,34]. The heat conduction is modeled as a weighable phonon gas flow passing through a porous medium. From the phonon gas viewpoint, the boundary scattering will terminate the mean free paths of both R processes and N processes. The reduction of λ_R can be interpreted as the variation of porosity, while the reduction of λ_N reflects the viscosity decrease as in rarefied gas dynamics. Accounting the above two effects simultaneously, the heat flux profile for the in plane heat conduction in a nanofilm is determined by [34]

$$\frac{\lambda_{R,\text{eff}}(z)}{\lambda_{R,0}}\kappa_0 \nabla T = -\mathbf{q}(z) + \frac{\lambda_{R,\text{eff}}(z)\lambda_{N,\text{eff}}(z)}{5}\nabla^2 \mathbf{q}(z), \tag{5}$$

where z is the distance from the central line (as shown in Fig. 1(a)), subscript 0 means the value measured in the bulk sized material and subscript eff means the local value measured in the nano-sized material. The local effective thermal conductivity is different
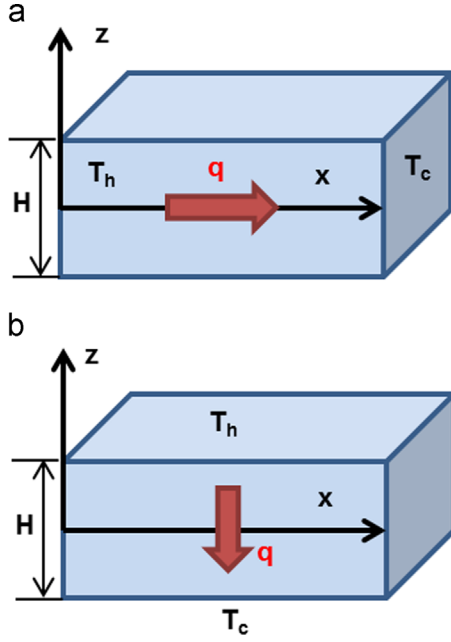
Fig. 1. (a) In-plane heat conduction of nanofilm; (b) cross-plane conduction of nanofilm. T_h means the hot end while T_c is the cold end.

from the bulk value, namely $\kappa(z)/\kappa_0 = \lambda_{R,\mathrm{eff}}/\lambda_{R,0}$. The effective mean free paths are obtained by assuming the boundary is purely diffusive, i.e. its emission is totally uncorrelated with the absorption. For nanofilms, one gets for the effective MFPs in analogy with the algorithm for microfluidics [34,36,37]

$$\frac{\lambda_{j,\mathrm{eff}}(z)}{\lambda_{j,0}} = 1 + \frac{1}{2}\left[(\alpha-1)e^{-\alpha} + (\beta-1)e^{-\beta} - \alpha^2 E_i(\alpha) - \beta^2 E_i(\beta)\right]. \qquad (6)$$

where

$$\alpha = \frac{H/2-z}{\lambda_{j,0}}, \quad \beta = \frac{H/2+z}{\lambda_{j,0}}, \quad E_i(\theta) = \int_1^\infty t^{-1} e^{-t\theta} \mathrm{d}t. \qquad (7)$$

with j representing R or N. With specified $\lambda_{R,0}$ and $\lambda_{N,0}$, Eq. (5) can be numerically solved and the effective κ for in plane conduction is obtained. In a previous paper [34], we use $\lambda_{R,0} = 42$ nm, which is the classical value based on Eq. (1), and $\lambda_{N,0} = 360$ nm, which is the optimum value for the both Si nanofilms and nanowires at room temperature and gives good agreement with the experiments. In general $\lambda_{N,0}$ depends on the branch and frequency of phonons. Here an average value of $\lambda_{N,0}$ is adopted to maintain the simplicity of this model. The first principle calculation [38] shows that at the room temperature the average value of $\lambda_{N,0}$ is several times larger than $\lambda_{R,0}$, which agrees with the present assumption.

3. Cross plane heat conduction model based on BTE

Compared with the in plane heat conduction, the experimental results for cross plane heat conduction in nanofilms are rare, since the contact resistance could be much larger than the film resistance. Nevertheless, there are some numerical results for this issue such as the MC and MD simulations, which also indicated the strong decrease of effective κ from the bulk value. Terris and coworkers [16] used three numerical methods, including kinetic theory of phonon gas, MC and discrete ordinate method, to calculate the cross plane conduction of Si nanofilm. They found the cross plane conductance is nearly constant in the sub-50 nm region. It means that the effective κ is a linear function of film thickness, H, and shrinks to zero when $H \to 0$. Feng, Wang and Li [39,40] carried out MD simulation for the cross plane κ of Si nanofilm. The linear size

dependence of effective κ is also observed, which is a similar behavior to the in plane conduction.

The collective transport of phonons is characterized by the phonon BTE, which generally has the form [19,29]

$$\left(\frac{\partial}{\partial t} + v_k^s(k)\nabla\right)f^s = Cf^s, \qquad (8)$$

where $f(k, x, t)$ is the distribution function of phonons, k is the wave vector, s is the index of phonon branches, v_k is the group velocity, $v_k = \partial\omega/\partial_k$, ω is the frequency, C is the collision operator. The macroscopic properties, namely internal energy density e and heat flux q, are obtained through the integral of f over the k space,

$$e = \sum_s \int_{\mathbf{k}} \hbar\omega^s f^s, \qquad (9)$$

$$q_i = \sum_s \int_{\mathbf{k}} \hbar\omega^s v_{k,i}^s f^s. \qquad (10)$$

To solve the BTE the collision operator C needs to be properly specified. In the following we do not write s and the summation over phonon branches is defaulted. The collision operator C is assumed to have a dual relaxation form [29]

$$Cf = -\frac{f-f_E}{\tau_R} - \frac{f-f_D}{\tau_N}, \qquad (11)$$

where τ_R and τ_N are the characteristic relaxation times of R and N processes, f_E is the Planck distribution for the thermal equilibrium state

$$f_E = \frac{1}{\exp(\hbar\omega/k_B T) - 1}, \qquad (12)$$

f_D is the displaced Planck distribution which conserves the phonon momentum

$$f_D = \frac{1}{\exp[(\hbar\omega - \hbar\mathbf{ku})/k_B T] - 1}, \qquad (13)$$

where u is the drift velocity of phonon gas. The contribution of N processes is neglected by many numerical solutions of BTE [10–16], where τ_R can be either a constant (gray approximation) or depend on temperature, frequency and polarization. If the R processes are rare, such as in pure crystals at low temperature, f is close to f_D, thus the effect of N processes can be reasonably neglected. In contrary, for materials at higher temperature, R processes are significant. Thus the distribution function deviates from f_D, and the second term on the left hand side of Eq. (11) (called Nf in following) should be accounted. A Chapman–Enskog expansion can be made to account the Nf term, which leads to the $\nabla^2 q$ term in Eq. (2) [29]. Therefore, the N processes also contribute to the thermal resistance when $f \neq f_D$ in the in-plane conduction problems. The effect of $\nabla^2 q$ term is only significant in small systems, where Kn is relatively large [20,21].

For the cross-plane conduction in nanofilms, the distance between the heat baths is too short to fully relax the phonon distribution function. The phonons emitted from one heat bath have a large chance to arrive at another side without scattering, namely transport ballistically. Thus the phonon distribution function can be far from f_D due to the ballistic transport, and the Nf term in Eq. (11) should be accounted. Chen established a Ballistic–Diffusive [41] heat conduction model by separately considering the ballistic part and diffusive part of phonon distribution function, which successfully characterizes the fast-transient heat conduction across thin films. The ballistic part originates from the boundary and attenuates to zero with a characteristic length, $v_s\tau$. The diffusive part obeys the BTE with a single relaxation collision term, thus the Nf term in Eq. (11) is neglected. For the steady state cross plane heat conduction, we also assume that the local distribution function can be separated into a ballistic part and a
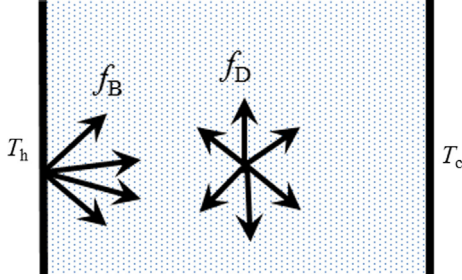
Fig. 2. The scheme of the ballistic–diffusive transport in cross plane direction.

diffusive part

$$f = f_B + f_d, \tag{14}$$

where f_B is the ballistic part emitted from the boundary, f_d is the diffusive part which is fully relaxed by the scattering, as shown in Fig. 2.

Guyer and Krumhansl [19,20] describe the picture of R and N processes as: The N processes do not break the total quasi-momentum of phonon gas, they just transfer the momentum between phonons to achieve a uniform drift. If the phonon gas already drifts uniformly, i.e. obeys the distribution of f_D, then the effect of N processes vanishes. For the one-dimensional heat conduction in bulk materials, the diffusive transport dominates. The phonon gas drifts uniformly with a constant heat flux. On the other hand, the transport region is far from the boundary compared with the MFP, thus the effect of N processes cannot exhibit. Therefore, we can approximate f_d in Eq. (14) by the displaced Planck distribution, f_D, in Eq. (13). It means that the diffusive part of phonon gas is not influenced by the N processes. This approximation is also adopted by Chen [41].

Inserting Eq. (14) into Eq. (10) one obtains

$$q = \int_k \hbar\omega v_k (f_B + f_D) = q_B + q_D, \tag{15}$$

where q_B and q_D are the heat flux contributed by f_B and f_D, respectively. Note that the heat flux here only means the energy flux passing through each cross-section. In very thin films the distribution function can highly deviate from the near equilibrium state and the state variables are ill defined. In one-dimensional transport the heat flux is constant in each location, thus q_B gets its maximum value at the boundary and decreases with the distance away from the boundary. Conversely, q_D is smallest at the boundary and increases continuously. The ballistic phonon distribution emitted from the boundary converts to the diffusive distribution with the distance away from the boundary due to the scattering processes. If the film is thick, the region where f_B is important is negligible compared to the whole system, so the phonon distribution is well approximated by f_D and the Fourier's law is recovered. In nanosystems, the ballistic region is non-negligible and the behavior of f_B is critical for the cross plane conductance.

Multiplying Eq. (11) with $\hbar\omega v_k$ and integrate it in k space yields

$$\frac{1}{3}\rho C_V v_s \frac{\partial T}{\partial z} = -\left(\frac{q_B}{\lambda_R} + \frac{q_B}{\lambda_N}\right) - \frac{q_D}{\lambda_R}. \tag{16}$$

If $q_B = 0$, i.e. in the diffusive limit, then Eq. (16) turns to

$$-\frac{1}{3}\rho C_V v_D \lambda_R \frac{\partial T}{\partial z} = q_D. \tag{17}$$

which is the Fourier's law with $\kappa = \rho C_V v_s \lambda_R / 3$. With this expression of κ Eq. (16) turns to

$$-\kappa \frac{\partial T}{\partial z} = q_D + q_B + \frac{\lambda_R}{\lambda_N} q_B = q + \frac{\lambda_R}{\lambda_N} q_B, \tag{18}$$

which shows q_B provides an additional resistance to the heat transfer. In this way, the normal process contributes to the thermal resistance if the phonon distribution contains a ballistic part. In the classical phonon theory the N processes do not contribute to the thermal resistance in bulk materials [35]. However, Ward and Broido [42] indicated that the N processes also contribute to the diffusive thermal conductivity in the first principle calculation. Tomas et al. [43] found that the collective thermal conductivity, which rises from both the N and R processes, is lower than the kinetic one, which rises from only the R processes. In our present derivation, the N processes provide additional thermal resistance in thin nanofilms where q_B plays an important role. This effect originates from the second term on the right hand side of Eq. (11).

To quantitatively evaluate the cross plane conductivity of nanofilms, the profiles of q_B and q_D need to be obtained. It can be inferred from Eqs. (11) and (16) that only R processes influence the diffusive heat flux, while both R and N processes attenuate the ballistic heat flux. Thus q_B loses momentum through both R and N processes. The R processes directly break the quasi-momentum, while the N processes take the momentum out of the ballistic distribution and convert it into the diffusive distribution. In this sense, the characteristic length for the conversion from q_B to q_D is λ_N. Assume the boundary is completely diffusive, i.e. $f_D = 0$ at the boundary, and remind that the total heat flux, q, is a constant, one obtains for the local value of q_B and q_D

$$q_B(z) = q\frac{\exp(-z/\lambda_N) + \exp(z/\lambda_N)}{\exp(-H/2\lambda_N) + \exp(H/2\lambda_N)} = q\frac{\cosh(z/\lambda_N)}{\cosh(H/2\lambda_N)}, \tag{19}$$

$$q_D(z) = q - q_B(x) = q\left[1 - \frac{\cosh(z/\lambda_N)}{\cosh(H/2\lambda_N)}\right]. \tag{20}$$

If we impose a unit flux q passing through the systems, the temperature drop can be decided through Eqs. (18)–(20). Then one gets the effective cross plane heat conductivity. Note that the mean free paths in Eqs. (18)–(20) are the local effective mean free paths, $\lambda_{R,\text{eff}}$ and $\lambda_{N,\text{eff}}$, calculated through Eqs. (6) and (7).

4. Anisotropy of Si nanofilms

We examine the anisotropy of Si nanofilms at room temperature for there are most experimental and theoretical results for comparison. The in-plane conductivity κ_x is calculated with Eq. (5) while the cross plane conductivity κ_z is calculated by Eqs. (18)–(20). The
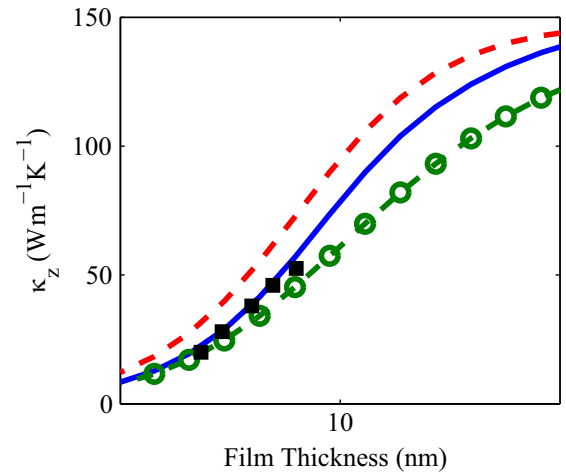

Fig.3. The size dependent cross-plane conductivity of Si nanofilm at room temperature. Present model calculated from Eqs. (18)–(20) (solid line), Gray model [17] (dashed line), McGaughy model [18] (dashed line with circle) and comparison with MD results [39,40] (square dots).
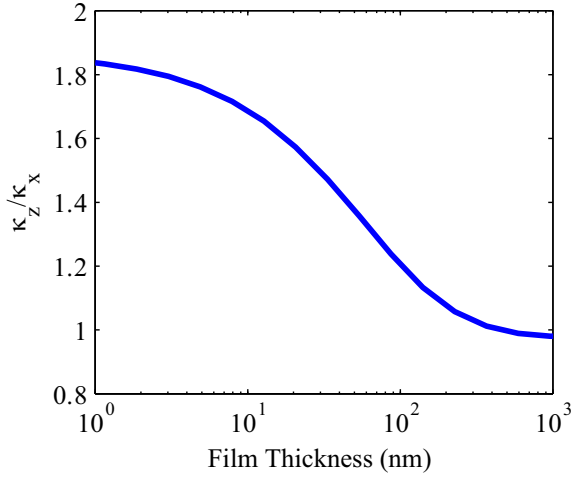
Fig. 4. The anisotropy of thermal conductivity vs. thickness of Si nanofilm at room temperature.

effective mean free paths are determined by Eqs. (6) and (7). The value of bulk mean free paths are chosen as $\lambda_{R,0} = 42$ nm, and $\lambda_{N,0} = 360$ nm. The size dependent cross plane conductivity κ_z of a Si nanofilm is presented in Fig. 3. The predictions of the Gray model [17] and McGuaghey model [18] are also shown in Fig. 3. The present model agrees well with the MD results by Feng, Wang and Li [39,40].

The anisotropy is defined as

$$A = \frac{\kappa_z}{\kappa_x}, \tag{21}$$

In Fig. 4 the dependence of A on the film thickness is presented. A has a maximum value of near 1.8 at the limit $H \rightarrow 0$, while reduces to 1 at the bulk limit.

The maximum anisotropy can be theoretically derived from the present model. It can be easily verified from Eqs. (6) and (7) that both $\lambda_{R,\text{eff}}$ and $\lambda_{N,\text{eff}}$, reduce to H at the limit $H \rightarrow 0$. In this case, the heat flux for the cross conduction is pure ballistic, i.e. q_B dominates. The effective thermal conductivity is extracted from Eq. (16)

$$\lim_{H \to 0} \kappa_z = \frac{H}{2} \frac{\kappa_0}{\lambda_{R,0}}. \tag{22}$$

For the in-plane conductivity, the effective conductivity is determined by Eq. (5) which turns to

$$\frac{H}{\lambda_{R,0}} \kappa_0 \nabla T = -\mathbf{q}(z) + \frac{H^2}{5} \nabla^2 \mathbf{q}(z), \tag{23}$$

The solution of Eq. (23) is

$$\lim_{H \to 0} \kappa_x = \frac{\kappa_0 H}{\lambda_{R,0}} \left[1 - \frac{2l_G}{H} \tanh\left(\frac{H}{2l_G}\right) \right] = \frac{\kappa_0 H}{\lambda_{R,0}} \left[1 - \frac{2}{\sqrt{5}} \tanh\left(\frac{\sqrt{5}}{2}\right) \right]. \tag{24}$$

It can be seen that at the ballistic limit, both κ_z and κ_x are linear to the film thickness, H, which agrees with the experimental and numerical results. Then the anisotropy at the thin film limit is

$$\lim_{H \to 0} \frac{\kappa_z}{\kappa_x} = \frac{1}{2 \left[1 - (2/\sqrt{5}) \tanh(\sqrt{5}/2) \right]} \approx 1.8. \tag{25}$$

At this time the effective viscosity of phonon gas is strongly reduced to the second order of H. Note that for κ_x, the diffusive resistance, which rises from the first term of Eq. (5), is still important. If one neglects this effect, Eq. (23) turns to

$$\frac{H}{\lambda_{R,0}} \kappa_0 \nabla T = \frac{H^2}{5} \nabla^2 \mathbf{q}(z). \tag{26}$$

Then one would have

$$\lim_{H \to 0} \kappa_x = \frac{5}{12} \frac{\kappa_0 H}{\lambda_{R,0}}, \tag{27}$$

which evidently overestimates the effective conductivity compared with Eq. (24).

5. Concluding remarks

In essence, the anisotropy of Si nanofilms is caused by the ballistic transport of phonons. The boundary scattering could be competitive with the phonon–phonon scattering in nanosystems. Therefore, the phonon distribution is not fully relaxed and the ballistic part of the phonon distribution should be considered. Based on the BTE with the dual relaxation approximation, Eq. (11), we see that if f deviates from f_D, then N processes also contribute to the thermal resistance. Such deviation is caused by the boundary scattering for nanofilms. For the in plane conduction, the main direction of ballistic transport from the boundary is perpendicular to the temperature drop, thus the contribution of N processes is accounted by the phonon viscosity effect, which can be evaluated by the Laplacian term of heat flux in Eq. (5). In this situation the phonon gas flow is analogous to a fully developed gas flow in a tube. For the cross plane conduction, the direction of ballistic transport from the boundary is parallel to the temperature drop, thus N processes also resist the heat flux if the phonon distribution is ballistic. It is in analogy with the entrance effect in fluid mechanics [27]. When the film thickness is much larger than the phonon mean free path, the ballistic region becomes negligible. Then the phonon transport is completely diffusive and the thermal conductivity turns isotropic. The present model, however, does not contain the quantum confinement effect of phonons. It is a reasonable simplification since the investigated system has a scale much larger than the characteristic wavelength of phonons, which is about 1.4 nm for silicon at room temperature [14,44].

It is notable that the boundaries of Si nanofilms are assumed to be pure diffusive in our model. It agrees with the presented experimental conditions or assumptions made in numerical models. In general cases the boundaries could be partly reflective or corrugated (which may cause back-scattering) regarding the production method. For the in plane heat conduction, the boundary condition could strongly affect the effective conductivity. If the boundaries become smoother, the κ_x will increase since boundary slip could happen. Conversely, if the boundaries are made rough, backscattering is possible to decrease κ_x. For the cross plane conduction, changing the couple strength with the heat bath could modify the ratio of f_B and f_D and consequently change the effective κ_z. It is expected that the anisotropy of κ is tunable depending on the boundary features of nanofilms such as roughness, heat treatment or deposited materials.

Acknowledgement

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