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Technical Note

Phonon ballistic-diffusive heat conduction in silicon nanofilms by Monte Carlo simulations

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ABSTRACT

An efficient Monte Carlo (MC) method on the basis of introducing a model of phonon scattering processes is proposed to simulate the ballistic-diffusive heat conduction in silicon nanofilms. The calculated thermal conductivity of nanofilms agrees with the experimental data, which is indicative of the validity of our simulations. The boundary temperature jump caused by the effects of phonon ballistic transport is observed by the MC technique. It is found that the boundary temperature jump increases with the Knudsen number (Kn). Theoretical models for predicting the boundary temperature jumps are also derived from the phonon Boltzmann transport equation. Model 1 is derived based on the acoustically thin approximation ($Kn \gg 1$), whereas model 2 is obtained by the diffusive approximation ($Kn \ll 1$). Furthermore, we derive model 3 in the intermediate region by an empirical way i.e. averaging model 1 and model 2. The theoretical models agree well with the MC simulations in different regions.

1. Introduction

Silicon (Si) is widely used to produce nanoscale wafers in electronics. The study on nanoscale heat conduction in silicon nanofilms is especially important. Heat conduction in silicon is predominant by phonons which are quanta of crystal vibrational energy [1]. In silicon nanofilms of which characteristic length is comparable to the phonon mean free path (MFP), some of phonons can directly fly from one boundary to another without scattering. It is called ballistic transport, causing heat conduction to deviate from the classical Fourier's law, such as the size dependence of thermal conductivity and the boundary temperature jump [2]. In the intermediate region, the transport of heat is known as ballistic–diffusive conduction and usually described by the Boltzmann transport equation (BTE) with the relaxation time approximation [3].

Great efforts have been devoted to study the ballistic-diffusive heat conduction in recent years. The size-dependent thermal conductivity has been obtained both in experiments [4] and theoretical analyses [5–7], which indicates the violation of the classical Fourier's law in nanoscale. Besides, the temperature profile in the ballistic–diffusive regime is also an important point. A temperature jump occurs at the boundary, which can be observed in the numerical solutions of the BTE [9,10] and the simulations of molecular dynamics (MD) [11] and Monte Carlo (MC) [13–17]. Jiang et al. [11] discussed the boundary temperature jumps in the MD simulations and analyzed the phonon edge modes which were regarded as the reason for the temperature jumps. Alvarez et al. [12] proposed that a thermal boundary resistance led to the temperature jump. However, the underlying mechanism of the boundary temperature jump is ambiguous and the model for predicting the boundary temperature jump is still lacking.

In the present work, we apply the MC technique to study the ballistic–diffusive heat conduction in silicon nanofilms at room temperature (300 K). We find that the effects of the phonon ballistic transport lead to the boundary temperature jump (BTJ) increasing with the Knudsen number. Furthermore, we derive the theoretical models for predicting the boundary temperature jumps based on the phonon BTE and compare them with the simulations.

2. Monte Carlo simulation details

The gray media approximation is used in our MC simulations. The gray media approximation assumes that the phonon properties are frequency-independent. By averaging the frequency-dependent phonon properties over the phonon population, the average phonon properties only depending on temperature can be calculated. Hence, in our simulations, phonons travel with one velocity and the scattering rate is approximated by one bulk average phonon MFP. Here, the bulk average phonon MFP, l_a, is calculated via the kinetic theory,

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Nomenclature

f	phonon distribution function
f_0	equilibrium distribution function
D	function of phonon density of states
e	phonon intensity per solid angle
l_a	mean free path
k_B	Boltzmann constant
L	thickness of nanofilm
N_p	number of phonon bundles
C_V	heat capacity at constant volume
v_g	average group velocity
$\mathbf{s}$	direction vector
x	spatial coordinate
V	volume
N	number of atoms
t	time
R	Radom number
E	hemispherical phonon intensity
T	temperature
q	heat flux
Kn	Knudsen number
W	energy per phonon bundle

Greek symbols

τ	relaxation time
σ	phonon Stephen Boltzmann constant
$\hbar$	Dirac constant
Θ_D	Debye temperature
θ	polar angle
φ	azimuthal angle
Ω	solid angle
ε	phonon emissivity
λ	thermal conductivity
ω_D	Debye frequency

Subscripts

bu	bulk
0	reference state
s	scattering
$-$	emitting into the boundary
+	emitting out from the boundary
θ_m	azimuthal angle in the media
θ_b	azimuthal angle at the boundary
φb	polar angle at the boundary
φm	polar angle in the media

$$l_a = \frac{3\lambda_{bu}}{C_V v_g}, \tag{1}$$

where λ_{bu} is the thermal conductivity of the bulk material, C_V is the heat capacity at constant volume and v_g is the average group velocity. As for silicon at room temperature, λ_{bu} is 150 W/(m K), C_V is 1.63×10^6 J/(m^3 K) and v_g is 6400 m/s [18]. Thus, the bulk average MFP is 43.7 nm. Arguments still exist on the value of the MFP of silicon at room temperature [8]. Based on a more detailed dispersion model and only considering acoustic phonons that carry most of heat, the MFP of silicon is about 260 nm [18]. However, it should be pointed out that when the longer MFP based on the dispersion model is chosen, the corresponding heat capacity and group velocity should also be changed. Here, the MFP is chosen as 43.7 nm with its corresponding heat capacity and group velocity. The similar choice was also taken in Ref. [10], in which the lattice Boltzmann method for phonon transport in silicon was reported.

The phonon intensity emitting into the media from a black-body boundary can be written as [2,17],

$$E = \sigma T^4. \tag{2}$$

Definition of the parameter, σ, known as the phonon Stephen Boltzmann constant is

$$\sigma = \frac{N k_B v_g \pi}{\Theta_D^3} \int_0^{\frac{\Theta_D}{T_0}} \frac{y^3}{\exp(y) - 1} dy, \tag{3}$$

where N is the number of atoms, Θ_D is the Debye temperature, T_0 is the reference temperature and k_B is the Boltzmann constant. Moreover, the phonon intensity emitting from a unit control volume, dV, in the media can be derived by the sort of mathematics used in the theory of participating media radiation [19]. The phonon intensity emitting from a unity volume in the media is written as

$$dQ_{em} = 4\varepsilon\sigma T^4 dV, \tag{4}$$

in which ε is the phonon emissivity ($\varepsilon = l_a^{-1}$). In a unit control volume, it is in equilibrium when the phonons received from the boundaries and all the other unit control volumes are equal to those emitting from this unit control volume. Based on the local thermal equilibrium assumption, the local temperature can be calculated.

The intensity of each phonon bundle emitting from the boundary is defined as

$$W = \frac{E}{N_p}, \tag{5}$$

where N_p is the number of phonon bundles that we trace. N_p must be large enough to preserve the simulation accuracy. The traveling direction vector of the phonon bundle is given by

$$\mathbf{s} = [\sin(\theta)\cos(\varphi), \sin(\theta)\sin(\varphi), \cos(\theta)]. \tag{6}$$

When the phonon bundle emits form the boundary, $\sin(\theta) = (R_{\theta b})^{1/2}$, $\varphi = 2\pi R_{\varphi b}$ ($R_{\theta b}$ and $R_{\varphi b}$ are independent random numbers ranging from 0 to 1). When the phonon bundle travels in the media, $\cos(\theta) = 1 - 2R_{\theta m}$, $\varphi = 2\pi R_{\varphi m}$ ($R_{\theta m}$ and $R_{\varphi m}$ are independent random numbers ranging from 0 to 1). The detailed derivation of the relations between the angles and independent random numbers can refer to Ref. [19].

During the transport process, phonons engage in various scattering events, which can be classified as phonon-interface scattering and intrinsic scattering. In our simulations, the boundaries are considered as black-body, so the phonons will be completely absorbed. A gray boundary with phonon absorptivity less than 1.0 will reflect phonons and make the reflected phonons travel in the opposite direction. Our simulations ignore this effect due to the black-body boundary assumption. The intrinsic scattering processes, such as phonon-impurities and phonon–phonon scattering, can be treated in the relaxation-time approximation [16]. Based on the relaxation time approximation, the traveling distance, Δl, can be calculated as [17]

$$\Delta l = -LKn \ln(1 - R_s), \tag{7}$$

where L is the characteristic length, Kn is the Knudsen number and $0 < R_s < 1$ is a random number.

The block diagram of our tracing algorithm is shown in Fig. 1. It shall be noted that our tracing algorithm is the one-bundle MC which is quite different from Refs. [14–16,23], where the tracing

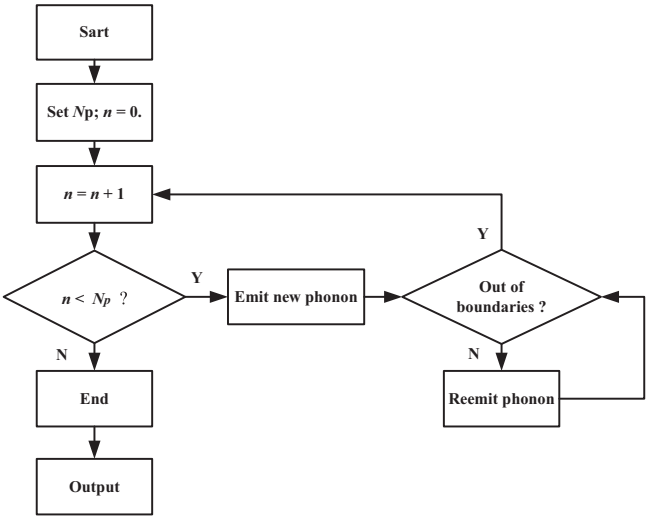

Fig. 1. Block diagram of our tracing algorithm.

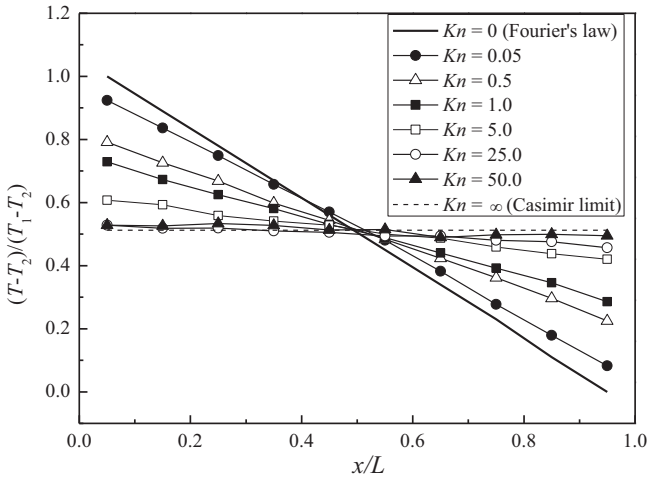

Fig. 2. Dimensionless temperature profiles of Si nanofilms.

algorithm is known as the ensemble MC [20]. In our tracing process, one phonon bundle is injected and its motion is traced in the domain, until it exits through the boundaries. Another phonon bundle is then injected and the process is repeated to simulate an ensemble of trajectories. As for the ensemble MC, instead of single phonon bundle, a large ensemble of phonon bundles is simulated at the same time. Comparing the two algorithms, the first has less computational expense and is simpler for simulating transient problems.

The simulation object is a monocrystalline silicon nanofilm with the thickness L. The physical properties of monocrystalline silicon at 300 K are shown in Table 1. In our simulations, the Knudsen number of the nanofilms ranges from 0.05 to 50. The two boundaries are maintained at temperatures of T_1 (305 K) and T_2 (295 K). The boundary temperature jump is defined as $T_1 - T(0)$, in which T_1 is the temperature of hot boundary and $T(0)$ is the average temperature of first cell of the discretization close to the hot boundary. The tracing number of phonon bundles is equal to 10^8.The thickness of unit control volume is $\Delta x = 0.1L$.

3. Results and discussion

The thickness-dependent thermal conductivity of Si nanofilms is calculated by the MC technique [17]. The MC simulations agree well with the experimental data, indicating that our simulations are properly handled. The dimensionless temperature profiles in Si nanofilms are shown in Fig. 2. The temperature profiles within the nanofilms are linear. As $Kn = 0$, the phonon transport is purely diffusive and the corresponding temperature profile can be calculated by the classical Fourier's law. With the increasement of the Knudsen number, phonon ballistic transport becomes stronger. The temperature jumps occur at the boundaries and the temperature gradient becomes smaller. As $Kn \to \infty$, since the phonon ballistic transport is dominant, the temperature gradient vanishes and the boundary temperature jump reaches the maximum value. Due to no phonon scattering in the nanofilm, the heat flux is $q_{\text{ballistic}} = \sigma(T_1^4 - T_2^4)$ and the temperature within the nanofilm is calculated as $T_{\text{ballistic}} = \left[\left(T_1^4 + T_2^4\right)/2\right]^{1/4}$. This is commonly known as the Casimir limit [6]. When the Knudsen number is equal to 50, almost no scattering events can occur in the nanofilm, and the temperature profile is very close to the Casimir limit. It is also found that the boundary temperature jump caused by the effects of ballistic transport increases with the Knudsen number. The models predicting the boundary temperature jumps can be derived based on the phonon BTE. The phonon BTE with the relaxation time approximation can be expressed as [2]

$$\cos(\theta) v_g \frac{df}{dx} = \frac{f_0 - f}{\tau}. \tag{8}$$

The phonon intensity per unit area and per solid angle is defined as [6]

$$e = \int_0^{\omega_D} v_g(\theta)\hbar\omega D(\omega) f d\omega, \tag{9}$$

where $D(\omega)$ is the Debye phonon density of states and ω_D is the Debye frequency [1]. The heat flux can be calculated as

$$q = \int e\cos(\theta) d\Omega. \tag{10}$$

Eq. (8) can be rewritten as

$$\cos(\theta)\frac{de}{dx} = -\frac{e}{\tau v_g} + \frac{1}{\tau v_g}\int_0^{\omega_D} d\omega v_g(\theta)\hbar\omega D(\omega) f_0. \tag{11}$$

According to Eqs. (2) and (3), we have [17]

$$\int_0^{\omega_D} d\omega v_g(\theta)\hbar\omega D(\omega) f_0 = \frac{\sigma T^4}{\pi}. \tag{12}$$

Substituting $Kn = v_g \tau/L = l_a/L$, we can obtain the phonon intensity transport equation

$$\cos(\theta) L\frac{de}{dx} = -\frac{e}{Kn} + \frac{1}{Kn}\frac{\sigma T^4}{\pi}. \tag{13}$$

Table 1
Physical properties of monocrystalline silicon at room temperature [21].

Specific heat	Thermal conductivity	Density	Average group velocity	Debye temperature	MFP
696 J/(kg K)	150 W/(m K)	2330 kg/m^3	6400 m/s	645 K	43.7 nm

According to the sort of mathematics used in solving the radiation transport equation in the participating media between two slabs [22], the temperature at location $x = 0$ can be expressed as,

$$T^4(0) = \frac{1}{2}\left(T_1^4 + T_2^4 \int_0^1 \exp\left(-\frac{1}{\cos(\theta)Kn}\right) d\cos(\theta) + \int_0^{1/Kn} \times \int_0^1 T^4(x) \exp\left(-\frac{x}{\cos(\theta)L}\right) d\cos(\theta)\left(\frac{dx}{\cos(\theta)L}\right)\right) \quad (14)$$

When $Kn \gg 1$, the acoustically thin approximation is applied. The nanofilm is regarded as nearly maintained at one same temperature, i.e. $T(x) = T(0)$. Expression (14) can be simplified as,

$$T^4(0) = \frac{T_1^4 + T_2^4 B(Kn)}{1 + B(Kn)}, \qquad B(Kn) = \frac{1}{Kn}\int_0^{Kn} \exp\left(-\frac{1}{z}\right) dz. \quad (15)$$

We can name Eq. (15) as model 1. Whereas, as $Kn \ll 1$, the diffusive approximation can be used, thus the phonon intensity per unit area and per solid angle is expanded as the Taylor series of Kn,

$$e = e^{(0)} + Kne^{(1)} + O(Kn^2). \quad (16)$$

Substituting Eq. (16) into the phonon intensity transport equation (13) yields

$$e^{(0)} = \frac{\sigma T^4}{\pi}, \qquad \cos(\theta)L\frac{de^{(0)}}{dx} = -e^{(1)}. \quad (17)$$

Thus,

$$e = e^{(0)} - Kn\cos(\theta)L\frac{de^{(0)}}{dx}. \quad (18)$$

The heat flux emitting out from the boundary whose temperature is maintained at T_1 is calculated as $q_+ = E(T_1)$. The heat flux emitting into the boundary is calculated as

$$q_- = 2\pi \int_{\pi/2}^{\pi} e\cos(\theta) d\cos(\theta). \quad (19)$$

Substituting Eq. (18) into Eq. (19) yields,

$$q_- = \sigma T^4(0) + \frac{2}{3}Kn\frac{d\left[\sigma T^4(0)\right]}{dx}L. \quad (20)$$

The net heat flux across the nanofilm is expressed as $q = q_+ - q_-$. Thus,

$$\sigma T_1^4 - \sigma T^4(0) = \frac{2}{3}Kn\frac{d\left[\sigma T^4(0)\right]}{dx}L + q. \quad (21)$$

Substituting Eq. (18) into Eq. (10), q can be calculated as

$$q = -\frac{4}{3}Kn\frac{d\left[\sigma T^4(0)\right]}{dx}L. \quad (22)$$

Thus,

$$\sigma T_1^4 - \sigma T^4(0) = -\frac{2}{3}Kn\frac{d\left[\sigma T^4(0)\right]}{dx}L. \quad (23)$$

We have,

$$\frac{d\left(\sigma T_1^4\right)}{dT_1}T_1 - \frac{d\left[\sigma T^4(0)\right]}{dT}T(0) = -\frac{2}{3}Kn\frac{dT(0)}{dx}\frac{d\left[\sigma T^4(0)\right]}{dT}L. \quad (24)$$

Since $Kn \ll 1$ and $d(\sigma T_1^4)/dT \approx d[\sigma T^4(0)]/dT$, Eq. (24) can be simplified as

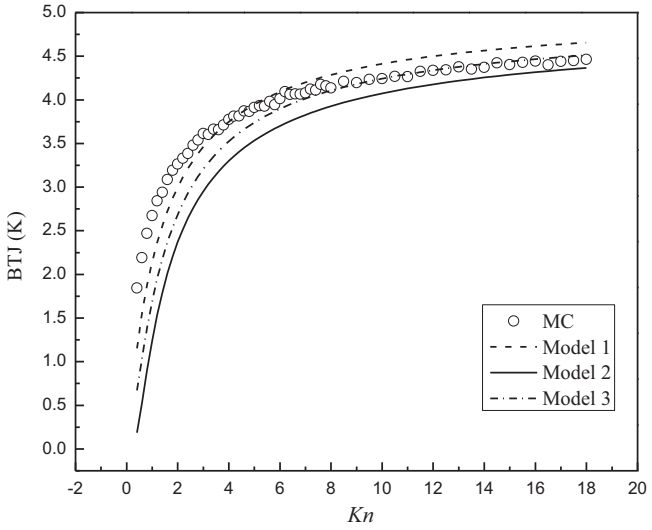

Fig. 3. Boundary temperature jumps vs. Knudsen number.

$$T_1 - T(0) = -\frac{2}{3}Kn\frac{dT(0)}{dx}L. \quad (25)$$

Eq. (25) is named model 2. In the nanofilm, the heat flux can also be calculated as [6],

$$q = \frac{4\sigma T_0^3(T_1 - T_2)}{\frac{3}{4Kn} + 1}. \quad (26)$$

Thus the BTJ can also be expressed as

$$T_1 - T(0) = \frac{T_1 - T_2}{\frac{3}{2Kn} + 2}. \quad (27)$$

The boundary temperature jumps by the MC simulations and theoretical models are shown in Fig. 3. As $Kn > 15$, model 1 based on the acoustically thin approximation is better fitting with the simulations. When $Kn \to \infty$, $T(0) = \left[\left(T_1^4 + T_2^4\right)/2\right]^{1/4}$ predicted by model 1 corresponds to the Casimir limit. Whereas, as $Kn < 5$, model 2 based on the diffusive approximation is better. As $Kn = 0$, the BTJ by model 2 vanishes corresponding to the classical Fourier's law. However, as $5 < Kn < 15$, neither model 1 nor model 2 can predict the BTJ by the simulations well, since this region is intermediate, and the assumptions of our models (acoustically thin approximation and diffusive approximation) are both invalid. It is found that in this intermediate region the BTJ calculated by the MC technique is just between model 1 and model 2. So the model to predict the BTJ in this region can be derived by a completely empirical way, i.e. averaging model 1 and model 2. Thus the boundary temperature can be given by,

$$T(0) = \frac{1}{2}\left\{T_1 - \frac{T_1 - T_2}{\frac{3}{2Kn} + 2} + \left[\frac{T_1^4 + T_2^4 B(Kn)}{1 + B(Kn)}\right]^{\frac{1}{4}}\right\}. \quad (28)$$

This empirical averaged model is named as model 3. The values calculated by model 3 are also shown in Fig. 3, which can agree well with the simulations in the intermediate region.

4. Conclusions

(1) We propose an efficient MC method based on establishing a model of phonon scattering processes. It is then employed to simulate the ballistic-diffusive heat conduction in silicon nanofilms. The calculated size-dependent effective thermal conductivity agrees well with the experimental data, which verifies the validity of our MC simulations.

(2) The MC technique is applied to study the boundary temperature jump caused by the effects of phonon ballistic transport. Our simulations show that the boundary temperature jump increases with the Knudsen number.
(3) The theoretical models,

$$\begin{aligned} &Kn > 15 && T^4(0) = \tfrac{T_1^4 + T_2^4 B(Kn)}{1 + B(Kn)}, \\ &5 \leqslant Kn \leqslant 15 && T(0) = 0.5\left\{T_1 - \tfrac{T_1 - T_2}{\frac{3}{2Kn} + 2} + \left[\tfrac{T_1^4 + T_2^4 B(Kn)}{1 + B(Kn)}\right]^{1/4}\right\}, \\ &Kn < 5 && T_1 - T(0) = -\tfrac{2}{3} Kn \tfrac{dT(0)}{dx/L}, \end{aligned}$$

for predicting the boundary temperature jumps in different regions are derived based on the phonon Boltzmann transport equation, and agree well with the MC simulations.

Conflict of interest

None declared.

Acknowledgments

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