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Effect of discrete number of velocity directions of phonon on thermal conductivity prediction in the cross-plane direction of superlattices

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ABSTRACT

In this paper, we analyze the effect of the discrete number of velocity directions of the phonon on thermal conductivity prediction in the cross-plane direction of superlattices based on solving the phonon Boltzmann transport equation (BTE) numerically. The simulation shows that the accuracy of the calculation is mainly affected by discretization number of polar angle (N_θ). To improve the efficiency in the two-dimensional situation, choosing a proper discrete number of velocity directions of the phonon can be used. Besides, the relationship between the control angle (M) and Knudsen (*Kn*) number is concluded when the relative error is less than 5%.

1. Introduction

In recent years, thermal conductivity of superlattice structures has attracted significant attention owing to the importance of different applications [1–7]. Due to the reduction of phonon thermal conductivity, many kinds of superlattices, such as Bi_2Te_3/Sb_2Te_3 [2] and PbTe/PbSeTe [8] quantum dot superlattices, have shown dramatic increase in thermoelectric figure of merit ZT [9,10] values compared to their bulk materials. The theoretical value of the thermal conductivity of the superlattices is calculated from the constituting single crystal materials based on the Fourier's Law of Heat Conduction. Several experiments [11-13] reveal that the experimental value is lower than the theoretical one. Moreover, the thermal simulation of superlattices is not perfect at present. The distribution and transmission of thermal energy in the lattice are often described by the Boltzmann transport equation (BTE), when the effects of coherent phonon transport are negligible [14,15]. Phonon distribution function is affected by several factors, such as space-time coordinates, wave vector as well as polarization, making fully-resolved simulation costly [14,16,17]. Thus, in order to solve the BTE, it is necessary to develop efficient and accurate numerical methods. In this work, we try to figure out the thermal conductivity of superlattice structures accurately and efficiently by simplifying the phonon velocity directions. The finite volume method (FVM) [18] as well as the discrete ordinates method (DOM) [14] is a common method. In comparison, the FVM is unaffected by the false scattering, and radiation effect is not obvious as well [19]. As regard to structured Cartesian grids, weights of the different angular direction is the main difference between the DOM and the FVM [14]. However, owing to the need of structured Cartesian grids, the DOM imposes a great trouble on the problems related to complex geometries. By contrast, the FVM is much more easily employed to unstructured grids.

Recently, FVM has been studied to numerically solve the BTE by many researchers. R. Yang and G. Chen [20] discussed the thermal conductivity prediction of Periodic Nanocomposites by employing the FVM. Y. Xu and G. Li [21] also employed the FVM to analyze the influence of the strain on phonon thermal conductivity of two-dimensional nanocomposite materials. H. Li, Y. Yu, and G. Li [22] also analyzed the thermoelectric properties of nanoporous silicon by using the FVM. SC. Mishra [23] discussed the compatibility and suitability of the lattice Boltzmann method (LBM) and the FVM, finding that there is no much difference between the two techniques in iteration number and CPU time. To meet accuracy, these works chose a larger discrete number of velocity directions, but will reduce the computational efficiency because the number is proportional to the simulation time in theory [20,21,23].

Considering the conditions above, we analyze the thermal conductivity of superlattices using the FVM and the LBM. The motivation of this work is to try to find the effect of discrete number of velocity directions on thermal conductivity prediction of superlattices.

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Nomenclature

c	volumetric specific heat, $J\,K^{-1}\,m^{-3}$
D	states density per unit volume, m^{-3}
f	phonon distribution function
$\hbar$	Planck constant divided by 2π, $J\,s^{-1}$
I	phonon intensity, $W\,m^{-2}\,s\,r^{-1}$
k	thermal conductivity, $W\,m^{-1}\,K^{-1}$
L	representative physical length scale, m
M	control angle M = Nθ × Nφ, rad^2
N	discretization number, rad
U	volumetric internal energy, J/m^{-3}
$\|V_{mi}\|$	magnitude of the phonon group velocity, ms^{-1}
X	coordinate
Y	coordinate
Z	coordinate
Λ	mean free path, m
υ	group velocity, ms^{-1}
ω	phonon frequency, Hz
ω_{max}	the cut-off frequency of each polarization, Hz
θ	polar angle, rad
φ	azimuthal angle, rad
μ	directional cosine
ζ	thickness
Kn	Knudsen number

Superscript

$*$	deviation

Subscripts

i	properties of i-th layer
θ	polar angle
φ	azimuthal angle
e	effective
m	polarization
x	coordinate
y	coordinate
z	coordinate

2. Theoretical model and computational procedure

2.1. Phonon Boltzmann equation

Knudsen number (Kn) is a significant dimensionless number describing the mechanism of phonon transport, which ranges from ballistic to diffusive. $Kn = \Lambda/L$, where Λ denotes phonon mean free path, L donates representative physical length scale and defines the thermal transport domain [14]. When Kn is much less than 1, the Fourier approximation is applicable, for diffusive effects are dominant. With the increase of Kn, the influence of bulk scatting becomes not that significant. In the meanwhile, the heat transfer is controlled by the phonon interactions with boundaries as well as interfaces. When Kn is bigger than 1 and the length scale of the system nearly equals the phonon mean free path, the BTE can be employed to the modeling of phonon transport [16,17,24]. Noting that, the phonon model can predict the thermal conductivity of superlattices well, we focus on the phonon transport in the cross-plane direction, by assuming that [20]: (1) the effect of phonon wave can be ignored. (2) the average phonon mean free path (MFP) is applied to approximately describe the frequency dependent scattering rate in the bulk medium. (3) the interface scattering is diffuse.

Based on the phonon distribution function, the general form of the phonon Boltzmann equation can be defined as [16,17,20,24]

$$I_i = \frac{1}{4\pi}\sum_m \int_0^{\omega_{\max}} |V_{mi}| f \hbar\omega D_{mi}(\omega) d\omega \tag{1}$$

where I is the total phonon intensity, subscript i (=1, 2) represents the i-th layer, $D(\omega)$ represents the state density per unit volume, f denotes the phonon distribution function, $\hbar$ is the Planck constant, $|V_{mi}|$ represents the absolute value of the phonon group velocity, ω represents the phonon frequency, ω_{max} represents the cut-off frequency of each polarization.

The first law of thermodynamics is used in the analytical process. Based on this, we acquire an expression for the equilibrium intensity [25]:

$$\begin{aligned} I_{0i}(x,y) &= \tfrac{1}{4\pi}\int_{4\pi} I_i(r,\Omega)d\Omega \\ &= \tfrac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} I_i(x,y,\theta x,y\sin\theta)d\theta d\varphi \end{aligned} \tag{2}$$

The single mode relaxation time approximation is used in this procedure. Based on this, we may get

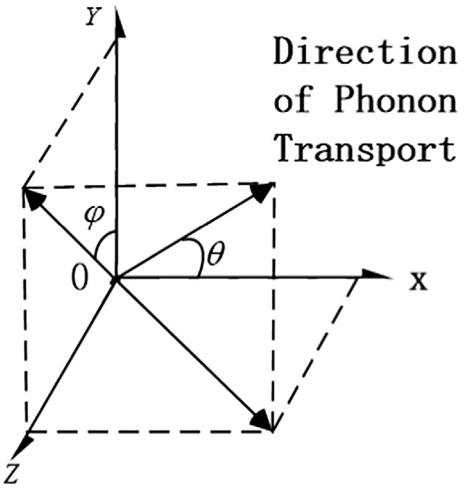

Fig. 1. Local coordinate used in phonon Boltzmann equation simulation.

$$\sin\theta_i\cos\varphi_i\frac{\partial I_i}{\partial y} + \cos\theta_i\frac{\partial I_i}{\partial x} = -\frac{I_i - I_{oi}}{\Lambda_i} \tag{3}$$

where θ and φ, as shown in Fig. 1, represent the polar angle and azimuthal angle, respectively. Λ represents the average phonon MFP.

In addition, Ref. [26] shows that MFP really suits the thermal conductivity modeling on cross-plane transport. Hence, considering the similarity of the two researches, frequency independent phonon MFP was also used in this study for the sake of simplicity.

2.2. Boundary and interface conditions

Owing to the non-physical accessional scattering at the boundaries, specified emitted temperature boundary condition may lead to man-made temperature jump at the boundaries [27]. In this work, the periodic boundary condition is used based on the fundamental physics of phonon transport in periodic structures [15].

The same phonon intensity distortion exists in every corresponding direction of each corresponding point on the boundary of x = 0 and x = L, which physically reflects the periodicity of the boundary condition [20].

The equation can be written as

$$I(L_{Si},y,\theta,\varphi) - I_0(L_{Si},y) = I(0,y,\theta,\phi) - I_0(0,y)$$