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The effective thermal conductivity of ballistic–diffusive heat conduction in nanostructures with internal heat source

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ABSTRACT

In nanostructures whose characteristic lengths are comparable to the phonon mean free path, the ballistic–diffusive heat conduction leads to the size effect, geometry dependence and anisotropy of the effective thermal conductivity. In the present work, we have studied the effective thermal conductivity of the ballistic–diffusive heat conduction in nanostructures (including nanofilms and nanowires) with internal heat source using Monte Carlo simulation and Boltzmann transport equation. It is found that the effective thermal conductivity of nanostructures with internal heat source is significantly lower than that with temperature difference, though it still increases with the increasing characteristic length. The models for the effective thermal conductivity and the temperature distribution of the cross-plane heat conduction in the nanofilms with internal heat source are directly derived from the phonon Boltzmann transport equation, and the comparisons with the Monte Carlo simulations well confirm their validities. As for the effective thermal conductivity of the in-plane nanofilms and nanowires with internal heat source, referring to the Matthiessen's rule, the models are in the form of $k_{eff}/k_{bulk} = 1/(1+\alpha Kn)$, with the parameter α obtained by the best fitting with the Monte Carlo simulations. Moreover, the diffusive heat conduction equation with the effective thermal conductivity can well characterize the temperature distributions in the in-plane nanofilms and long nanowires, while it fails in the short nanowires due to the influence of the axial constraints.

1. Introduction

Wide applications of semiconductor nanostructures in electronics and photonics require further understanding of heat transport at nanoscale [1]. Phonons predominate the heat transport in semiconductors [2]. For nanostructures whose characteristic lengths are comparable to the phonon mean free path (MFP), owing to the ballistic transport and the phonon-boundary scattering, heat conduction deviates from the Fourier's law which corresponds to the limit of completely diffusive transport. The presence of both the ballistic and diffusive transports leads to the ballistic–diffusive heat conduction which is usually characterized by the phonon Boltzmann transport equation (BTE) with the relaxation time approximation [3],

$$\vec{v}_g \cdot \nabla f = \frac{f_0 - f}{\tau} + \dot{S}_\Omega, \tag{1}$$

where $\vec{v}_g$ is the group velocity, f is the phonon distribution function, f_0 is the equilibrium distribution function, τ is the relaxation time, and $\dot{S}_\Omega$ is the phonon source per solid angle. In the ballistic–diffusive regime, some of phonons can directly travel from one boundary to another without internal scattering events, and the influence of the phonon-boundary scattering becomes remarkable. Essential indications for the ballistic–diffusive heat conduction include the size effect, geometry dependence and anisotropy of the effective thermal conductivity [4–6].

Studies on the effective thermal conductivity of nanostructures have been conducted both theoretically [7–15] and experimentally [16–21]. It has been found that in the ballistic–diffusive regime the effective thermal conductivity, which significantly reduces as compared to the bulk material, increases with the increasing characteristic length and varies with the direction of heat flow. In modeling researches [7,8], a nanostructure is generally assumed to be in contact with two heat sinks of different temperatures and the temperature difference induces the heat flow. Then using the Fourier's law the effective thermal conductivity is calculated out. On the basis of the temperature difference (TD) scheme stated above, the theoretical models of the effective thermal conductivity have been derived from the phonon BTE [7–9,22]. Besides the TD scheme has been widely adopted in simulations [11,12] and experiments [4,16,17]. Actually, the TD scheme is not the only choice for the thermal

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Nomenclature

f	phonon distribution function
f_0	equilibrium distribution function
DOS	function of phonon density of states
l	mean free path
c_V	volumetric specific heat
v_g	average group velocity
Kn	Knudsen number
k	thermal conductivity
T	temperature
T^*	dimensionless temperature
q	heat flux
$\dot{S}_\Omega$	phonon source per solid angle
L	length of nanowire
D	diameter of nanowire
L_x	x-directional thickness of nanofilm
L_y	y-directional thickness of nanofilm
$\dot{S}$	internal heat source

Greek symbols

τ	relaxation time
$\hbar$	Dirac constant
θ	polar angle
ω	angle frequency
ρ	mass density
φ	azimuthal angle
η	dimensionless coordinate

Subscripts

0	reference state
cr	cross-plane
in	in-plane
T	temperature difference scheme
I	internal heat source scheme
$film$	nanofilm
$wire$	nanowire

conductivity measurements. The internal heat source (IHS) scheme has also been used in experiments [18–21]. The internal heat source is introduced in the nanostructures and the resulting temperature rise is measured; then the effective thermal conductivity is obtained by comparing the measuring result with the analytical solution of the diffusive heat conduction equation. Liu and Asheghi [18] measured the in-plane thermal conductivity of silicon layers by introducing a steady-state uniform internal heat source (Joule heating), while the theoretical model obtained from the TD scheme was employed to analyze the experimental data. In the experiments of Johnson et al. [20], a transient internal heat source was introduced via diffraction of a laser beam to measure the thermal conductivity of the free-standing silicon membranes. In addition, the IHS scheme has also been a useful tool for the thermal conductivity measurements of carbon nanotubes [1,21].

Although both the TD and IHS schemes have been widely adopted for the thermal conductivity measurements, it is still ambiguous whether the effective thermal conductivity obtained by the TD scheme is the same as that by the IHS scheme, in particular for the ballistic–diffusive heat conduction. Li and Cao [13,14] studied the effective thermal conductivity of the nanostructures with internal heat source by the non-equilibrium molecule dynamics simulations, and found that the effective thermal conductivity in the IHS scheme was significantly lower than that in the TD scheme. Phonons emit from the heat sinks at boundaries in the TD scheme, while in the IHS scheme phonons originate within the media, and the different phonon emitting locations can lead to different boundary confined effects on phonon transport. Phonons originating within the media undergo more boundary-scatterings than these emitting from the heat sinks at the boundaries, and the mean free path (MFP) in the IHS scheme can be more confined by the boundaries than in the TD scheme [13]. According to the kinetic theory [2], the effective thermal conductivity is proportional to the boundary-confined MFP. Therefore, the effective thermal conductivity in the IHS scheme is significantly lower than that in the TD scheme. Moreover, in the electronic devices where self-heating does exist, the accurate prediction to the effective thermal conductivity of nanostructures with internal heat source becomes highly essential. Although the heat transport in electronic devices has been widely studied [23,24], the theoretical model for the effective thermal conductivity of the nanostructures with internal heat source is still lacking. Therefore the size-dependent behavior of the effective thermal conductivity in the nanostructures with internal heat source still remains poorly understood, and the predictive model is highly desired.

In the present work, the effective thermal conductivity of the nanostructures (including nanofilms and nanowires) with internal heat source is studied. A Monte Carlo (MC) technique is applied to simulate the phonon transport. It is found that the effective thermal conductivity in the IHS scheme is significantly lower than that in the TD scheme. The predictive models for the effective thermal conductivity of the nanostructures with internal heat source are derived based on the phonon BTE and the Matthiessen's rule. Moreover, the diffusive heat conduction equation with the effective thermal conductivity is applied to characterize the temperature distributions in the nanostructures with internal heat source.

2. Analyses and simulation details

2.1. Internal heat source (IHS) scheme

The IHS scheme is illustrated in Fig. 1(a.1)–(c.1). A steady-state uniform internal heat source $\dot{S}$ is introduced in the nanostructures in contact with two heat sinks of the reference temperature T_0. The cross sectional boundaries are adiabatic. Therefore, in the diffusive limit, the heat conduction can be regarded as one-dimensional, and the temperature profile is derived from the Fourier's law,

$$T(x) = \frac{\dot{S}}{2k}(L_x - x)x + T_0, \tag{2}$$

where L_x is the distance between the two heat sinks, and k is the thermal conductivity. Particularly, for the in-plane nanofilms as shown in Fig. 1(b.1) and the nanowires as shown in Fig. 1(c.1), the temperature $T(x)$ is averaged in the cross-section area. The effective thermal conductivity is then extracted from the mean temperature increase $\Delta\bar{T}$ of the nanostructures

$$k_I = \frac{L_x^2 \dot{S}}{12\Delta\bar{T}}, \tag{3}$$

with

$$\Delta\bar{T} = \frac{1}{L_x}\int_{L_x} T dx - T_0. \tag{4}$$