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Ballistic-diffusive heat conduction in multiply-constrained nanostructures

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ABSTRACT

Ballistic-diffusive heat conduction in multiply-constrained nanostructures is theoretically studied based on the phonon Boltzmann transport equation. The results show that different constraints influence the thermal transport in different ways. In the direction parallel to the heat flow, the phonon ballistic transport can cause temperature jumps at the boundaries in contact with the phonon baths. In contrast, for lateral constraint, the heat flux is reduced near the boundaries due to phonon-boundary scattering. A thermal conductivity model for multiply-constrained nanostructures is then derived from the phonon Boltzmann transport equation. The influences of different constraints are combined on the basis of Matthiessen's rule. The model accurately characterizes the thermal conductivities of various typical nanostructures, including nanofilms (in-plane and cross-plane) and finite length nanowires of various cross-sectional shapes (e.g. circular and rectangular). The model predictions also agree well with Monte Carlo simulations and experimental data for silicon nanofilms and nanowires.

1. Introduction

The rapid development of nanotechnologies necessitates an in-depth understanding of nanoscale thermal transport [1]. At the macroscale, the transport in the diffusive limit corresponds to the classical Fourier's law, $q = -k\nabla T$, where q is the heat flux, T is the temperature and k represents the thermal conductivity which is an important intrinsic property of all materials. For nanomaterials in which the heat carrier mean free path (MFP) is comparable to the characteristic length, the ballistic transport and boundary scattering make the thermal conductivity dependent on the nanostructure geometry and size, indicating a violation of Fourier's law [2–11]. The presence of both diffusive and ballistic transport mechanisms leads to ballistic-diffusive heat conduction [12]. The interest in the size-dependent thermal conductivity of semiconductor nanostructures in the ballistic-diffusive regime has been growing owing to their many applications in electronics and photonics [1].

For semiconductor materials (e.g. silicon), phonons dominate the thermal transport. In the ballistic-diffusive regime, phonon transport is characterized by the phonon Boltzmann transport equation (BTE) with a relaxation time approximation

$$v_g \cdot \nabla f = \frac{f_0 - f}{\tau}, \tag{1}$$

in which f is the phonon distribution function, f_0 is the equilibrium distribution function, v_g is the phonon group velocity and τ is the relaxation time. The influence of the boundaries is not directly seen in Eq. (1) but is seen in the imposed boundary conditions, with different boundary conditions having different influences on the thermal transport. Theoretical studies of the size-dependent thermal conductivity have been conducted especially for nanostructures with only simple boundary constraints, such as nanoflims (in-plane or cross-plane) [13–16] and nanowires with particular cross sectional shapes and infinite lengths [17–19]. Engineering systems generally have more than one constraint on the nanostructures, e.g. finite length nanowires used in experiments [20,21]. The experiments of Chen et al. [20] showed that the thermal conductivities of silicon nanowires were mainly dependent on the diameter, since the nanowires were several microns long. In contrast, the experiments of Hsiao et al. [21] demonstrated that the thermal conductivities of silicon-germanium nanowires were strongly correlated with the length but not the diameter. Although

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Alvarez and Jou [15,22] proposed a model considering multiple constraints by introducing an effective characteristic length, the influences of the different constraints on the thermal transport were not identified in their model. The size and geometry dependence of the thermal conductivity in multiply-constrained nanostructures is still poorly understood and a general characterization of their thermal conductivities is needed. Present work theoretically studies the ballistic-diffusive heat conduction in multiply-constrained nanostructures based on the phonon BTE. The influences of different constraints on the thermal transport have been clarified and a phonon thermal conductivity model is given for multiply-constrained nanostructures. The model characterizes the thermal conductivities of various typical nanostructures, including nanofilms (in-plane and cross-plane) and finite length nanowires of arbitrary cross-sectional shapes.

2. Thermal conductivity model of multiply-constrained nanostructures

Fig. 1 shows a representative geometry of multiply-constrained nanostructure. This geometry can reduce to other typical nanostructures, including nanofilms (cross-plane and in-plane) and nanowires with varied cross sections. The left and right sides are in contact with the hot (T_1) and cold (T_2) phonon baths. The heat flux, q, caused by the temperature difference is along the x-direction. The length in this direction is denoted by L_x. The lateral boundaries are adiabatic and the phonons scatter at them with a specular scattering rate p. The thermal conductivity is related to both the longitudinal length, L_x, and the size and geometry of the cross section.

The thermal conductivity of the multiply-constrained system can be calculated by solving the phonon BTE. However, an analytical solution of the phonon BTE is rather difficult to obtain when simultaneously considering all the constraints. Another way to solve this complicated problem is to deal with the constraints separately. Their effects on the thermal conductivity are then combined based on Matthiessen's rule. In the longitudinal direction (x-direction) parallel to the heat flow, the ballistic transport of the phonons can cause temperature jumps at the boundaries [23], which will reduce the thermal conductivity, while for the lateral constraint, the phonon-boundary scattering reduces the heat flux near the boundaries which reduces the thermal conductivity. Therefore, different methods should be used for different constraints.

2.1. Longitudinal constraint

First consider the longitudinal constraint. The corresponding one-dimensional BTE is,

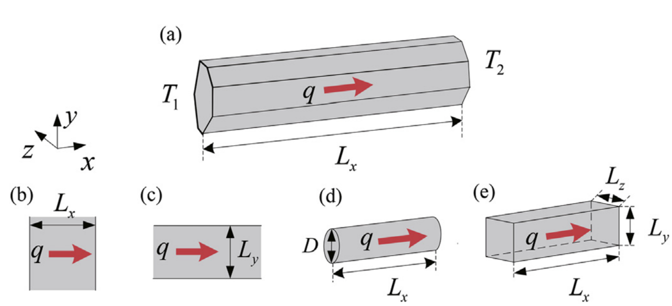

Fig. 1. Representative geometry of a multiply-constrained nanostructure (a). It can typically reduce to: (b) a nanofilm (cross-plane), (c) a nanofilm (in-plane), (d) a circular nanowire, and (e) a rectangular nanowire.

$$\mu l_0 \frac{\partial f}{\partial x} = f_0 - f, \tag{2}$$

where $\mu = \cos(\theta)$ in which θ is the polar angle between the phonon motion direction and the x-axis and l_0 is the bulk MFP equal to $v_g\tau$. For this case, Majumdar [13] proposed the gray model based on the differential approximation, but it is invalid for large Knudsen number. Here, the gray model was improved by dividing the distribution function into two parts, $f = f_b + f_d$, where f_b is the ballistic part directly originating from the boundaries and f_d is the diffusive part described by the differential approximation. This methodology was first proposed by Ofle [24] for calculating radiation heat transfer and Chen [12] then applied it to model transient ballistic-diffusive heat conduction.

The ballistic distribution function is given by,

$$\mu l_0 \frac{\partial f_b}{\partial x} = -f_b. \tag{3}$$

The ballistic heat flux, q_b, is then,

$$q_b = 2\pi\left[\int_0^1 \exp\left(-\frac{x}{\mu l_0}\right)\mu d\mu I_{w1} - \int_0^1 \exp\left(-\frac{L_x - x}{\mu l_0}\right)\mu d\mu I_{w2}\right] \tag{4}$$

with

$$I_{w1} = \varepsilon I_{01} + 2(1-\varepsilon)\int_0^1 \exp\left(-\frac{L_x}{\mu l_0}\right)\mu d\mu I_{w2}, \tag{5}$$

$$I_{w2} = \varepsilon I_{02} + 2(1-\varepsilon)\int_0^1 \exp\left(-\frac{L_x}{\mu l_0}\right)\mu d\mu I_{w1}, \tag{6}$$

in which ε is the phonon emissivity, $I_{01} = \int v_g \hbar\omega f_0(T_1) DOS(\omega) d\omega = \rho c_v v_g T_1/(4\pi)$ and $I_{02} = \int v_g \hbar\omega f_0(T_2) DOS(\omega) d\omega = \rho c_v v_g T_2/(4\pi)$ where $DOS(\omega)$ is the density of states, c_v is the volumetric specific heat and ρ is the mass density. For convenience, define the exponential integral function $E_n(t) = \int_0^1 \exp(-t/\mu)\mu^{n-2} d\mu$ and the ballistic heat flux as,

$$q_b = 2\pi\left[I_{w1} E_3\left(\frac{x}{l_0}\right) - I_{w2} E_3\left(\frac{L_x - x}{l_0}\right)\right]. \tag{7}$$

The diffusive distribution function is governed by,

$$\mu l_0 \frac{\partial f_d}{\partial x} = f_0 - f_d. \tag{8}$$

The differential approximation of Eq. (8) yields

$$q_d = q - q_b = \frac{1}{3}\rho c_v v_g l_0 \frac{\partial T_d}{\partial x}, \tag{9}$$

with the Marshak boundary conditions [25].

$$T_d(0) - \frac{4l_0}{3}\left(\frac{1}{\varepsilon} - \frac{1}{2}\right)\frac{\partial T_d(0)}{\partial x} = 0, \tag{10}$$

$$T_d(L_x) + \frac{4l_0}{3}\left(\frac{1}{\varepsilon} - \frac{1}{2}\right)\frac{\partial T_d(L_x)}{\partial x} = 0, \tag{11}$$

in which q_d is the diffusive heat flux and T_d is defined as $T_d = \frac{2\pi}{\rho c_v v_g}\int_{-1}^{1} d\mu \int \hbar\omega v_g f_d DOS(\omega) d\omega$. The boundary conditions