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A Monte Carlo simulation for phonon transport within silicon structures at nanoscales with heat generation

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ABSTRACT

Nanoscale phonon transport within silicon structures subjected to internal heat generation was explored. A Monte Carlo simulation was used. The simulation procedures differed from the current existing methods in which phonons below a predefined "reference temperature" were not accounted to reduce memory storage and computational resources. Results indicated that the heat diffusion equation significantly underestimates temperature distribution at nanoscales in the presence of an external heat source. Discussions on temperature distribution inside silicon thin film when heated by a pulsed laser, an electron beam or due to near-field thermal radiation effects were also provided.

1. Introduction

At macroscales, the rate of heat conducted through an area is proportional to the thermal conductivity and the temperature gradient, following the Fourier law [1–4]. The basic premise of the law is that the characteristic length of the object must be greater than the mean free path of the heat carriers. Using this phenomenological law to represent heat fluxes on all the surfaces of an object, the heat diffusion equation can be derived by simply summing all these fluxes and equating them to the rate of change of its internal energy. Even though the Fourier law is generally applicable at the macroscales, it is commonly used at the microscales to represent thermal heat flux of electrons and phonons [2,5–9]. For example, in the ultra-fast heating of metallic films where highly non-equilibrium phenomena is observed, the two-temperature model (TTM) is used to simulate thermal conduction of electrons and phonons [9–11]. The TTM basically consists of two coupled diffusion equations where heat fluxes of electrons and phonons are calculated separately. This formulation is also employed in the electron–phonon hydrodynamic equation (EPHDEs) to express the thermal flux of electrons and the heat flux of phonons as a function of corresponding thermal conductivity and temperature gradient [2,9,12]. However, when the characteristic length of an object is smaller than the mean free path, which is commonly observed at nanoscales, heat conduction no longer obeys the Fourier law, mainly due to the impact of ballistic propagation by the heat carriers. At such scales, thermal conductivity and temperature gradient are reduced while discontinuity in the temperature distribution near the boundary exists [13–20]. Therefore, either the general Boltzmann transport equation (BTE) or the phonon radiative transport equation (PRTE) is required to correctly model the phonon transport [1,2,21–26]. The energy equations for electrons and phonons in the TTM and the EPDHEs where the diffusion approximation is assumed are to be substituted by the corresponding BTE in the intensity form in order to account for the ballistic behaviors of heat carriers. This can be done only when the average mean free path of electrons/phonons exceeds the physical length of the system. Typical electron and phonon mean free paths range from 1 to 500 nm depending on the wavelength and energy [1,2,23,27]. An object with characteristic dimensions less than the mean free paths would generally exhibit (semi-) ballistic behavior.

Among analytical and numerical methods available to solve the BTE [1,2,4,23,26,28], Monte Carlo (MC) simulations are proven to

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Nomenclature

c_v	speed of light in vacuum [m/s]
D	density of states [m^{-3}-s]
E	energy [eV]
f	particle distribution function [–]
$\dot{g}'''$	power density/volumetric heat generation [W/m^3]
g_{sl}	Weyl component of the dyadic Green's function between layers s and l [m]
i	complex constant, $(-1)^{1/2}$ [–]
k	wavenumber [m^{-1}]
k_T	thermal conductivity [W/m-K]
k_B	Boltzmann's constant [eV/K]
N	number of phonons or ensembles [–]
N_b	number of division in phonon frequency domain [–]
p	polarization branch [–]
P	probability [–]
R	cumulative probability distribution function [–]
Ran	a random number [–]
S	distance of interaction [m]
T	temperature [K]
t	time [s]
v_g	group velocity [m/s]
X	width of the geometry [m]
Y	length of the geometry [m]
Z	depth (or thickness) of the geometry [m]

Symbols

μ	direction cosine [–]
τ	relaxation time [s]
Θ	mean energy of a Planck oscillator, J
β	parallel component of the wavevector [rad/m]
γ	perpendicular component of the wavevector ($= \gamma' + i\gamma''$) [rad/m]
ε_r	dielectric function ($= \varepsilon_r' + i\varepsilon_r''$)
ρ, θ, z	polar coordinate system
ω	angular frequency [rad s^{-1}]

Subscripts

$*$	complex conjugate
0	equilibrium
E	electric
en	ensemble
gen	heat generation
H	magnetic
ini	initial
LA	longitudinal acoustic
m	medium
ph	phonon
ref	reference
TA	transverse acoustic
ω	monochromatic

be the most flexible and accurate, yet they can be slow and expensive in terms of computational resources depending on the levels of physics included in the simulation. Many researchers have used MC simulations for phonon transport at nanoscales because of its flexibility in accounting complicated geometries and the correct phonon dispersion relation and different polarization branches [14,16–20,25,29–31]. While the simulation has been successfully used for predicting thermal conductivities of nanostructures such as nanowires and nanofilms [14,18–20,31–34], there is plenty of room for improvement in the algorithm, especially for treating the phonon–phonon scattering mechanisms. On the other hand, the effect of external heat generation on phonon transport near ballistic limit has never been studied, which is the focus of this work.

To explore phonon transport at nanoscales, here we introduce a new MC simulation procedure to solve phonon transport within a 3D-rectangular geometry, as depicted in Fig. 1. The model is a rectangular system ($X \times Y \times Z$) where constant temperature is applied at both ends along the Z-dimension while the other surfaces are assumed insulated. Depending on the dimensions of ($X \times Y$), the geometry can be considered as a Z nm thin film with infinite X and Y, a nanorod with comparable magnitudes of X, Y, and Z, or a nanowire where $Z >> X$ and Y. The 2D top view of the geometry is also provided in Fig. 1 to illustrate phonon activities during the transport process. Phonons are emitted from the constant temperature boundaries while additional phonons are generated within the medium/material as a result of external heating. We do not prescribe the type of external heating in the simulations because this is irrelevant as long as the heating process directly produces energetic phonons corresponding to the amount of the volumetric heat generation specified. The constant temperature boundaries are assumed to be perfect absorbers. In the simulations, the insulated surfaces along the Z-dimension can be of specular or diffusive type. As the names implied, a specularly insulated surface acts like a mirror while a diffusive insulated surface reflects phonons diffusively upon encountering. Reflection in the latter can be regarded as the effect of surface roughness.

In the following sections, a modified MC simulation procedure used in this formulation is first explained in detail including all the phonon scattering properties and algorithms for determining scattering processes of phonons. These procedures are general and can be adapted for simulating phonon transport in any material; in this work we explicitly use the properties of silicon. Simulations for other materials will be carried out in another study. The MC simulations are verified against known analytical solutions at the ballistic and diffusive limits. Next, the impacts of ballistic phonon transport on temperature distribution are studied for different heat generation distributions. Finally, we provide discussions and potential future works on the applications of the MC results coupled with near-field thermal radiation, laser heating, or electron-beam heating.

2. A modified Monte Carlo simulation in phonon transport

A typical MC simulation strategy for phonon transport is relatively straight forward: we initialize, launch, and trace phonon ensembles in terms of temperature, frequency, polarization, and positions. Local temperature distribution varies depending on the positions of these ensembles. A general flowchart of the MC simulation is shown in Fig. 2. The simulation starts by initializing all the phonon ensembles (including those to be launched from the constant-temperature boundary and within the material due to heat generation at each Δt). These ensembles are moved ballistically from one position to another within the time interval of Δt, assuming that ensemble properties remain unaltered. Ensembles that hit a constant-temperature boundary are recorded in terms of energy for heat flux calculation and then deleted. Those that encounter an insulated surface are assumed to be reflected specularly or diffusively. Otherwise, ensembles reside at the corresponding locations after the ballistic movement. Once the propagation phase is complete, local temperature distribution is calculated based on the positions of the ensembles. It is important to notice that local phonon distribution function after the propagation phase is different from the equilibrium distribution (i.e., the Bose–Einstein distribu-