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Sub-continuum thermal transport modeling using diffusion in the Lattice Boltzmann Transport Equation

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ABSTRACT

The Boltzmann Transport Equation is employed to model one-dimensional heat conduction problems at sub-continuum scales. A semi-gray Lattice Boltzmann (LB) model is presented and validated against a diffusive model of steady state thin film heat conduction with temperature boundary conditions. The size-dependent effective thermal conductivity curves of a gray LB model and a semi-gray LB model for Silicon are generated. In addition, a new semi-gray LB model with diffusion term is applied to determine the effective thermal conductivity. The transient features and dimension concerns of the new semi-gray LB model are also investigated. Results demonstrate that the semi-gray LB model with a diffusion term successfully recovers the size-dependent data of effective thermal conductivity and matches well with the diffusive solution valid at large scales. This approach can be applied to improve the accuracy of thermal modeling on micro-scale electronic systems.

1. Introduction

Generation by generation, Silicon-on-Insulator (SOI) transistors have been scaled to smaller sizes (∼200 nm) with higher frequencies to improve the speed and functionality of electronic devices [1]. It has been discovered that the traditional Fourier heat equation fails in thermal prediction for nanoscale structures, where the continuum assumption is invalid. At sub-continuum scales, the effective thermal conductivity appears much lower than the bulk value, as the mean free path of the energy carriers becomes comparable with the characteristic length of the heat transport domain [2]. In the sub-continuum regime, phonons as the energy carriers behave ballistically, which leads to a non-equilibrium energy distribution and localized temperature. The Boltzmann Transport Equation (BTE) is widely used in the analysis of heat transport via phonons in the sub-continuum region [1,3]. For most studies, the wave effect of electrons and phonon frequency dependence are neglected. The Lattice Boltzmann Method (LBM) has been proven to be an efficient approach to solve the BTE and can be extended to solve multi-dimensional problems [4–6]. A refined LBM approach is presented by Pisipati [7], where a diffusive term is introduced to eliminate the non-equilibrium temperature discontinuity.

Many experimental works have been performed to help understand the effective thermal conductivity of Si thin films with multiple sizes. Ju [8] measured the in-plane thermal conductivity of monocrystalline films as thin as 74 nm to derive the mean free path of thermal phonons at room temperature. Liu [9] provided the thermal conductivity of self-heated silicon between 300 and 450 K for thicknesses down to 20 nm.

Several approaches based on two BTE models are developed to simulate thermal transport with sub-continuum sizes: the gray model and semi-gray model. The gray model considers a single propagation mode of phonons with linear dispersion relationship, while the semi-gray model includes one propagating mode and one reservoir mode [6]. Distinct mean free paths and phonon velocities are employed in each model to match bulk material properties. Comparison with experimental measurements shows that the gray LBM considerably underestimates the size effect on thermal conductivity. This is due to the fact that the gray approximation neglects phonon dispersion [8]. Mansoor [10] employed the equation of phonon radioactive transfer (EPRT) model to govern energy transport in adjacent dielectric thin films, where solid-angle-averaged energy intensity is applied to describe temperature. A new type of heat conduction equations is derived by Chen [11] to solve transient heat conduction applicable from nanoscales to macroscales. In Chen's study, the heat flux is attributed to two components: one originates from the ballistic nature of boundaries, and the other is generated by diffusive transport from energy carriers. Pisipati [12] introduces an additional diffusive heat

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Nomenclature

C	volumetric heat capacity (J m^{-3} K^{-1})
D_p	density of states
e	phonon energy density (J m^{-3})
e^0	equilibrium phonon energy density (J m^{-3})
f	phonon distribution function
f^0	equilibrium phonon distribution function
g	phonon generation rate
$\hbar$	Planck constant divided by 2π (Js)
k	thermal conductivity (W m^{-1} K^{-1})
k_B	Boltzmann Constant (JK^{-1})
Kn	Knudsen number
L	characteristic length (m)
p	polarization
q_v, Q_v	volumetric heat generation rate (W m^{-3})
t	time (s)
T	temperature (K)
v	phonon velocity (m/s)
x	dimensional length

Greek symbols

α	thermal diffusivity (m^2 s^{-1})
δ	fraction of propagation phonon
λ	phonon mean free path (m)
θ_D	Debye temperature (K)
η	number density of phonons
τ	phonon mean free time (s)
ω	phonon frequency (Hz)

Subscripts

bulk	bulk value
c	low temperature side
0BTE	for Boltzmann Transport Equation
eff	effective
h	high temperature side
i	direction
P	propagation mode
R	reservoir mode
ref	reference
v	volumetric

Superscripts

0	equilibrium
$*$	dimensionless

flux term to refine the LBM, solving multi-layer thin film thermal transport problems. Studies based on the semi-gray BTE treat the longitudinal acoustic phonons as the sole moving carrier in thermal transport. The semi-gray BTE assumes instantaneous energy transport from electrons to phonons, and divides phonons into two modes: the propagation mode with higher velocities accounting for heat transfer, and the reservoir mode with lower velocities as energy storage [13]. The fraction of each mode is determined by the respective energy capacity at identical temperatures. Validated against measurement data, the semi-gray BTE provides more accurate size-dependent thermal conductivities of Si than the gray BTE [8]. A number of works based on the semi-gray BTE are performed on the thermal analysis of nanoscale transistors [14–17].

Meanwhile, information about the mean free path and relaxation time of phonons, which is critical in determining the thermal conductivity, remains incomplete. Traditionally the mean free path λ in the gray BTE is obtained by kinetic theory [18], $\lambda = 3\,k/Cv$, which yields the mean free path varying between 31–43 nm for silicon, based on the bulk thermal conductivity value. In consideration of phonon dispersion, the semi-gray BTE requires a much longer mean free path (200–300 nm) to recover the bulk thermal conductivity at room temperature. The specific value can be derived by an analysis of the semi-gray BTE solution and experiment data [8]. These mean free paths are determined from corresponding models, and are highly dependent of their respective assumptions. In recent years, several experimental studies [19,20] presented the phonon mean free path distribution spectrum of silicon over a wide temperature range. These studies indicate that phonons with mean free paths larger than the nanoscale significantly contribute to the thermal conductivity.

In this paper, a semi-gray BTE formulated in terms of lattice energy density with and without a diffusion term is introduced to model the one-dimensional heat conduction problem. Both steady and transient trace of the temperature/energy density distributions are computed for two types of heat conduction cases: (i). heat conduction with temperature gap at sides; (ii) identical boundary temperature with internal heat generation. The size-dependent effective thermal conductivities for silicon are obtained by the gray LBM and the semi-gray LBM with/without a diffusion term, and are compared over multiple scales. In current cases, only constant temperature boundary condition is discussed. For the gray LBM and semi-gray LBM without a diffusion term, the emitted phonon boundary conditions [7] are adopted for each boundary condition, i.e. specifying the energy density of phonons entering the domain. Previously in Pisipati's study [7] the total phonon energy boundary condition, which specifies the total energy density, was also presented and failed to demonstrate the size effect. Therefore it is neglected here. Both the gray and semi-gray LBM are compared with the Fourier solution for Kn = 0.01, which is within the diffusive region. Furthermore, a modified semi-gray LBM is introduced to reduce the governing variables and therefore the computational effort. Comparison is presented for the original and simplified semi-gray LBM over various sizes. Modeling results indicate that the steady state solution is not affected, while the transient difference depends on the size. A diffusion term is added to the semi-gray LBM and the steady/unsteady information is obtained for the two types of heat conduction problems. As the fraction of each phonon mode is temperature dependent and varies for different materials, the propagation rate-dependent behavior of the semi-gray LBM with diffusion is also studied. For the current study, phonon frequency dependence and interaction among different frequencies are neglected. Particularly with the semi-gray BTE, assuming the velocity or relaxation time of the reservoir phonons is negligible, thus ignoring the energy transport by reservoir mode, the propagation phonons are treated as the sole energy carrier [13]. Instead of the distribution spectrum, constant scalars are assigned to the mean free path and relaxation time of propagation phonons, and are derived by the traditional kinetic theory. Discrepancies occur in the semi-gray LBM model without diffusion.

2. One Dimensional BTE without diffusion

2.1. Gray Lattice Boltzmann Equations

As the quanta of lattice vibration, phonons are the primary energy carriers in semiconductor devices. The propagation and