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Finite element analysis of transient ballistic–diffusive phonon heat transport in two-dimensional domains

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ABSTRACT

While sub-continuum heat conduction becomes more important as the size of micro/nanodevices keeps shrinking under the mean free path of heat carriers, its computation still remains challenging to the general engineering community due to the lack of easily accessible numerical simulation tools. To address this challenge, this article reports the finite element analysis (FEA) of transient ballistic–diffusive phonon heat transport in a two-dimensional domain using a commercial package (COMSOL Multiphysics). The Boltzmann transport equation under the gray relaxation-time approximation was numerically solved by discretizing the angular domain with the discrete ordinate method (DOM) and the spatial domain with the FEA. The DOM-FEA method was validated by comparing the results with different benchmark studies, such as the equation of phonon radiative transfer, the ballistic–diffusive equation, and the finite difference method of the phonon Boltzmann transport equation. The calculation of phonon heat transport for a 2-D square slab reveals that heat conduction becomes more ballistic with temperature jumps at boundaries as Knudsen number (Kn) increases. The ballistic nature also significantly affects transient thermal behaviors at high Kn numbers. The obtained results clearly demonstrate the capability of the DOM-FEA as a promising engineering tool for calculating sub-continuum phonon heat transport.

1. Introduction

For the last two centuries, the conventional Fourier heat conduction equation has been used for modeling a diffusive nature of macroscale heat conduction by considering the energy conservation and Fourier's linear approximation of heat flux. However, it cannot accurately predict heat transport when the length scale is comparable to or smaller than the mean free path of thermal energy carriers or when the time scale is shorter than the carrier relaxation time [1–4]. When considering phonons as the dominant energy carrier of heat conduction, the Boltzmann transport equation (BTE) for phonons, or equivalently the equation of phonon radiative transport (EPRT), has been implemented to predict phonon heat transport in the sub-continuum space and time domains [5,6]. Majumdar's group [7,8] was the first who derived the EPRT from the BTE and proved its analogy with the radiative transport equation (RTE). By calculating the temperature profile and heat flux in a thin film from the one-dimensional (1-D) EPRT, they showed that the EPRT can describe a ballistic feature of phonon heat transport for the sub-continuum spatial and time scales. The EPRT has been also used to calculate the thermal boundary resistance across the interface of a thin film on a substrate [9], across interfaces of superlattices [10], and across mesoscopic constrictions at cylinder–substrate and sphere–substrate interfaces [11]. Narumanchi et al. [12] solved the transient two-dimensional (2-D) BTE under the gray relaxation-time approximation to study the effect of an unsteady, localized hot spot to phonon heat transport. In the following work, they considered frequency-dependent interactions between transverse and longitudinal acoustic phonons and optical phonons to incorporate more realistic phonon dispersion relations in silicon thin films [13]. The transient 1-D BTE with frequency- and polarization-dependence was also solved in Ref. [14] to better understand how phonon mean free paths can be extracted from the transient thermoreflectance experiment.

It should be noted that the BTE is inherently difficult to solve, particularly when the full physics of phonon dispersion and scattering is to be considered, due to its integro-differential formulation. However, the analogy between the phonon BTE (or EPRT) and the RTE has allowed the extension of several numerical

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Nomenclature

C	volumetric heat capacity (J/K-m^3)
D_p	phonon density of state (m^{-3})
e_0^*	nondimensional emissive power
e''	directional energy density (J/m^3 Sr)
e_0''	equilibrium energy density (J/m^3)
E_n	exponential integral
f	phonon distribution function
f_0	phonon distribution function at equilibrium
H	height of the 2-D domain (m)
Kn	Knudsen number
L	length of the 2-D domain (m)
$\hat{\mathbf{n}}$	outward-pointing normal from the domain
q''	heat flux (W/m^2)
$\hat{\mathbf{r}}$	position vector
$\hat{\mathbf{s}}$	direction vector
t	time (s)
T	temperature (K)
v_g	phonon group velocity (m/s)
w	weight function of Gaussian quadrature

Greek symbols

θ	polar angle (rad)
Θ	dimensionless temperature
Λ	phonon mean free path (m)
τ	relaxation time (s)
μ	directional cosine
ξ	optical thickness
φ	azimuthal angle (rad)
ω	angular frequency (s^{-1})
Ω	solid angle (Sr)

Subscripts and superscripts

b	boundary
m	azimuthal angle distribution
n	polar angle distribution
p	phonon
r	direction
SS	steady state

schemes originally developed to solve the RTE to the computation of the phonon BTE [5]. Such methods include the finite volume method (FVM) [11–13,15–17], the finite element analysis (FEA) [18–20], and the finite difference method (FDM) [7,8,14,21], combined with the discrete ordinate method (DOM) for angular discretization. In addition, the ballistic–diffusive approximation of the BTE has been introduced to alleviate computational complexities in directly solving the BTE while conveying the ballistic–diffusive features of phonon heat transport [21–24]. The advancement of computing power has also allowed the implementation of computation-intensive numerical methods, such as the molecular dynamics (MD) [25,26], Monte Carlo simulation [27–30] and the lattice Boltzmann method [31–33]. Recently, Yamada et al. [34] applied the dissipative particle dynamics with energy conversion, a coarse-grained MD simulation, to simulate heat conduction in a thin film with a less computational cost than the MD.

Although significant advances have been made in computing sub-continuum heat transfer, most of the aforementioned numerical approaches are not readily accessible to the general engineering community. It often requires too much time and effort to develop a home-built code, preventing the routine computation of sub-continuum phonon heat transport for the reliable design of micro/nanodevices and their performance evaluations. To overcome this challenge, the present study implements a commercial FEA package, COMSOL Multiphysics, to numerically solve the 2-D transient BTE. Although the COMSOL package has been used to compute the BTE [19,20], their works have been restricted to 1-D thin films. Since the BTE has a directional dependence, the DOM was combined to discretize the BTE in the angular direction [21]. The details of the numerical scheme are described in the consecutive section. In the results and discussion, the DOM-FEA is verified by comparing the numerically obtained temperature distribution along the centerline of a long rectangular domain with the semi-analytical solution of the 1-D EPRT [2]. The obtained results for 2-D geometry are also compared with DOM-FDM and ballistic diffusive equations (BDE) results from Ref. [21]. We also discuss steady and transient temperature distributions and related heat fluxes in a 2-D square slab for a wide range of Knudsen numbers, when an illustrative boundary condition has a hot temperature on the top surface while the other surfaces remain at a cold temperature.

2. Computation model

It is well known that phonons follow the Bose–Einstein statistics and interact with other phonons, electrons, and defects via scattering processes. Since BTE can model the statistical distribution of particle interactions via short-range forces, it is a valid and useful tool for studying classical size effects on phonon transport. In general, the BTE is a complicated nonlinear integro-differential equation and can be simplified with the gray relaxation-time approximation [5]:

$$\frac{\partial f}{\partial t} + \mathbf{v}_g \cdot \nabla f = \frac{f_0 - f}{\tau} \tag{1}$$

where f is the frequency-dependent distribution function of phonons, v_g is the averaged phonon group velocity, f_0 is the equilibrium distribution function, and τ is the effective relaxation time due to all phonon-scattering processes. The equilibrium distribution function of phonons follows the Bose–Einstein distribution, $f_0 = 1/[\exp(\hbar\omega/k_BT) - 1]$, where $\hbar$ is the reduced Planck constant, ω is the angular frequency, k_B is the Boltzmann constant, and T is temperature. It should be noted that the right-hand side of the equation denotes gray phonon-scattering with a single phonon velocity v_g in all directions and a single phonon relaxation time τ. Despite its simple form, the gray relaxation time approximation has proven to provide insight on phonon transport behaviors with an acceptable accuracy [11,13]. The BTE can be formulated with the phonon energy density as [5,35]

$$\frac{\partial e''}{\partial t} + \nabla \cdot \left(v_g \hat{\mathbf{s}} e''\right) = \frac{e_0'' - e''}{\tau} + \dot{q}_{vol} \tag{2}$$

The directional phonon energy density at position $\mathbf{r}$ and in direction $\hat{\mathbf{s}}$ (J/m^3-Sr) is defined as

$$e''(\mathbf{r}, \hat{\mathbf{s}}, t) = \sum_p \left(\int_0^{\omega_D} D_p(\omega) f \hbar\omega d\omega \right) \tag{3}$$

where $D_p(\omega)$ is the phonon density of state, ω_D is the Debye cutoff frequency, and the subscript p is the phonon polarization. The generation term $\dot{q}_{vol}$ represents the phonon source term due to electron–phonon scattering [21]. The phonon energy density at equilibrium, e_0'', can be determined from the following equation: