International Journal of Heat and Mass Transfer 127 (2018) 303–318

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

A three-dimensional phonon energy transport model based on the non-dimensional lattice Boltzmann method

Yan Su [a,*], Jane H. Davidson [b]

[a] Department of Electromechanical Engineering, FST, University of Macau, Taipa, Macau
[b] Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN 55455, USA

ARTICLE INFO

Article history:
Received 9 May 2018
Received in revised form 26 June 2018
Accepted 28 June 2018

Keywords:
Knudsen numbers
Lattice Boltzmann method
Phonon transport
Size effect

ABSTRACT

A new three-dimensional phonon energy transport model based on the non-dimensional lattice Boltzmann method (NDLBM) is developed to be applicable in the sub-continuum regime for diffusive and ballistic phonon transport. Two Knudsen numbers based on the base frequency and variable frequency, Kn_{ω_0} and Kn_{ω}, are defined in order to isolate the effects of material size and phonon transfer frequency. Both the relaxation time and boundary conditions of the phonon Boltzmann transport equation are modeled in dimensionless form. The physical meaning of each component in the relaxation time and discontinuous boundary models is interpreted. By introducing the Boltzmann constant and Planck's constant, all other coefficients can be simplified into order of one. The transient dimensionless phonon probability distribution functions are solved by the Parallel NDLBM with D3Q27 grids. The dimensionless temperature distributions, i.e. the dimensionless phonon energy density distributions, compare favorably with previous experimental and numerical results for various Kn_{ω_0}. The effects of material size, temperature, and phonon transfer frequency are investigated.

1. Introduction

Phonon energy transport has received more and more attention with the increasing importance of the sub-continuum length scale heat transfer in applications of microelectronic devices [1–4]. Phonon energy transport through a thin nanofilm structure or a nanowire structure based on the phonon Boltzmann equation has been studied for more than two decades [5,6]. In the early work, either experimental methods [7,8], or computational methods based on molecular dynamics [9–11] or Monte Carlo technique [12,13] were used to obtain the effective heat conductivity. After obtaining the effective heat conductivity, the ratio curve of the effective heat conductivity (k_{eff}) to the bulk heat conductivity (k_b) was fit based on the linear relationship $k_{eff}/k_b = 1/(1 + \beta Kn)$, where Kn is the Knudsen number (Kn), and β is a constant [14]. Then, the correlation of k_{eff} with Kn was applied to solve the macroscopic or integral form of the governing equation to obtain the temperature distributions in a space, i.e., the phonon energy distributions along the transportation direction [14–16]. However, these early studies do not consider the effects of the transient local temperature distribution on the local heat conductivity. Also, they do not solve the phonon Boltzmann equation with transient local relaxation time directly.

Direct solution of the phonon Boltzmann equation is a challenging problem. Some researchers [17,18] employed the finite difference or finite element method to solve it. However, the computational costs are extensive, especially for transient 3D simulations. Therefore, most of the previous studies focus on 2D stimulations. Recently, a mesoscopic computational method named Lattice Boltzmann Method (LBM) was developed in the field of computational fluid dynamics [19]. LBM can dramatically increase the computational speed for flow in complex geometries [20,21], phase change heat transfer with transient interfaces [22], and multiple phase multiple component flow problems [23–26]. Some recent applications of LBM to simulate phonon transfer include references [27,28]. Uniform weighting factors based LBM for the equilateral hexagon grid D2Q7 and the Gaussian grids D2Q9 and D3Q15 have been applied in phonon transfer simulations [27,28]. Nabovati et al. [27] show that when equal weights are applied, the Gaussian quadrature grid D2Q9 has a lower accuracy compared to the isotropic D2Q7 grid. This lower accuracy might be due to the fact that the weighting factors for D2Q7 equilateral hexagon grids are inherent uniform, while the weighting factors for Gaussian quadrature grids D2Q9 and D3Q15 are inherent non-uniform.

Two factors are key in solving the phonon transport equations by LBM. One is the modeling of the relaxation time, and the other

* Corresponding author.
E-mail address: yansu@umac.mo (Y. Su).

https://doi.org/10.1016/j.ijheatmasstransfer.2018.06.148
0017-9310/

Nomenclature

c_p	fixed pressure specific heat capacity, J/kg K
c_v	fixed volume specific heat capacity, J/kg K
c_s	lattice speed of sound, m/s
c	mesoscopic velocity scale, m/s
$\mathbf{c}$	discrete mesoscopic velocity vector, m/s
E	phonon energy density, J/m^3
f	phonon distribution function, K
k	thermal conductivity, W/mK
Kn	the Knudsen number
Kn_ω	varying frequency Knudsen number
Kn_{ω_0}	base frequency Knudsen number
L	macroscopic length scale, m
Ma	Mach number
q	heat flux, W/m^2
t	time, s
T	temperature, K
v	phonon transfer velocity, m/s
w	weighting factor
x, y, z	coordinates
$\mathbf{x}$	coordinates in vector form

Greek symbols

δ	distance from boundary, m
ΔT	temperature scale, K
Δx	lattice size, m
λ	effective mean free path, m
Λ	wave length, m
α	thermal diffusivity, m^2/s
β	a ratio constant
η	a ratio factor
ν	frequency, Hz
ρc_v	volumetric specific heat capacity, J/m^3 K
τ	effective relaxation time, s
ω	angular frequency, rad/s
ℓ	mesoscopic length scale, m

Subscripts

a	direction index
b	block value
eq	equilibrium state
eff	effective values
g	group values
$high$	higher value
(i,j,k)	index of coordinates
a	index of discrete velocity directions
od	opposite direction
ℓ	mesoscopic length scale
low	lower value
L	macroscopic length scale
ref	reference
w	wall
ω	effective values at frequency ω
ω_0	effective values at frequency ω_0
0	base values
$\pm$	forward and backward directions

Superscripts

$\_$	space averaged value
$*$	dimensionless variables

is the modeling of the boundary temperature jump. Due to the difficulties in isolating the effects of many governing parameters, the relaxation time models and their empirical coefficients have been defined in various forms [27,28]. Empirical coefficients are usually applied to adjust coefficients in the numerical models to match the analytical or experimental results. The previous LBM models for the phonon probability distribution functions due to temperature jump are not presented clearly in the sense that they lack of physical interpretations. A function linearly rated to Knudsen number is usually applied to adjust the coefficients in the relaxation time model. These previous LBM models cannot clarify the relative strength of the specular and diffuse reflections. The decompositions of the effective relaxation time of previous models differ to a great extent in both the format and their empirical coefficients. Clearly, the empirical coefficients matched from some particular cases may not be applied in other settings. Therefore, these boundary condition models have limited applicability in practice. Moreover, the effective heat conductivity and heat flux are mainly affected by the relaxation time model, while the discontinuous boundary temperature jump is mainly affected by the boundary condition model of phonon distribution function. Also the changing patterns of temperature jump may not always be the same as that of heat conductivity and heat flux.

The above limitations of previous studies in the available literature motivate us to generate a uniform non-dimensional lattice Boltzmann model for phonon energy transfer. In the present study, both dimensionless relaxation times and discontinuous boundary conditions for the phonon transport equation are modeled with physics-driven parameters and coefficients. The three-dimensional temperature, heat conductivity, and heat flux distributions are illustrated by using parallel NDLBM simulations with D3Q27 Gaussian quadrature grids. A full map of study of the effects due to material size, temperature and frequency on the boundary temperature jump, effective relaxation time, heat conductivity, and heat flux is presented.

2. A non-dimensional phonon lattice Boltzmann model

2.1. The Boltzmann transport equation for phonon distribution function

Denote f as the phonon distribution function. The Boltzmann transport equation with relaxation time τ is given by [5] as,

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \frac{f^{eq} - f}{\tau} + S, \tag{1}$$

where S is a heat source term. Note that f is a function related to multiple variables such as phonon frequency, space, and time. The relaxation time τ is also the mean free time between scattering [5]. In the present model, we use the mesoscopic length scale, $\ell = \Delta x$, temperature scale $\Delta T = T_{high} - T_{ref}$, and mesoscopic velocity scale $c = c_s/c_s^*$, where c_s is the lattice sound speed, and c_s^* is the dimensionless lattice sound speed ($c_s^* = 1/\sqrt{3}$ [19]). Also, we set the lattice sound speed to the phonon group velocity, i.e., $c_s = v_g$. Phonons dominating heat transport travel at the speed of sound [5]. Hence, the mesoscopic time scale is $\Delta t = \ell/c$.

With these scales, the dimensionless Boltzmann transport equation with f^* as the dimensionless phonon distribution function can be obtained as,

$$\frac{\partial f^*}{\partial t^*} + \mathbf{c}^* \cdot \nabla f^* = \frac{f^{eq*} - f^*}{\tau^*} + S^*. \tag{2}$$