A ballistic-diffusive heat conduction model extracted from Boltzmann transport equation

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A ballistic-diffusive heat conduction model is derived from the Boltzmann transport equation by a coarse-graining approach developed in the present study. By taking into account of the lagging effect, this model avoids the infinite heat propagation speed implied by the classical Fourier law. By expressing the heat conductivity as a function of the Knudsen number, it accounts for the size effect of the nanoscale heat conduction. The variation of the obtained effective heat conductivity with respect to the characteristic length shows an agreement with the experimental results for thin silicon films and nanowires in the nanoscale regime.

Keywords: heat conduction; Boltzmann transport equation; size effect; silicon film; silicon nanowire

1. Introduction

Recent decades have witnessed the rapid development of nanotechnology. With continuing progress in miniaturization technology, more and more nanoscale devices are now being created. The investigation of their thermal, mechanical and electrical properties has caught enormous attention. The experimental and numerical results show that the heat conduction of nanoscale devices demonstrates some distinct features from that of their macroscale counterparts, such as the size and memory effects. Therefore, there is a growing demand for scientific understanding of the nanoscale heat transport phenomena.

The Fourier law is fundamental to the classical heat transfer theory. However, it is well recognized that this law is not applicable to the heat transport of nanoscale devices whose size is comparable or smaller than the mean free path of the heat carriers (Brorson et al. 1987; Joshi & Majumdar 1993; Tzou 1996; Chen 2001; Cahill et al. 2003; Fujii et al. 2005). Many efforts have been devoted to the modification of the Fourier law. Joshi & Majumdar (1993) developed an equation of phonon radiative transfer that can be employed to model the ballistic to diffusive phonon transport. Chen (2001) established a non-Fourier heat conduction model from the Boltzmann transport equation (BTE) and applied it to the transient ballistic and diffusive heat conductions in thin films.

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Naqvi & Waldenstrom (2005) proposed a non-Fourier heat conduction equation in which the thermal conductivity is time dependent and related to the Knudsen number.

Recently, a non-Fourier heat conduction model was proposed by Alvarez & Jou (2007, 2008) with the aim of describing the heat transport from the ballistic to the diffusive regimes, in which the thermal conductivity is dependent on the Knudsen number, thus it captures the size effect of the nanoscale heat conduction. The theoretical basis of this model is the extended irreversible thermodynamics, which was developed by making the Maxwell–Cattaneo law of heat conduction compatible with the second law of thermodynamics (Jou et al. 1999, 2010). Unfortunately, Christov & Jordan (2005) found that the Maxwell–Cattaneo law violates Galileo’s principle of relativity.

For energy transports at micro- or nanoscale levels or under extremely short transient heating times, the BTE is usually employed to model the electron or the phonon transport. However, even the BTE under the relaxation time approximation still contains too much information of motions of energy carriers to be handled. Therefore, it is of great importance to extract the macroscale transport properties of materials from the BTE by coarse-graining processes which allow us to bridge the gap between microscopic and macroscopic descriptions of transport phenomena. Several approaches for the reduced description of the BTE are available: the Hilbert method (Hilbert 1912), the Chapman–Enskog method (Enskog 1917; Chapman & Cowling 1970), the Grad moment method (Grad 1949) and the invariant manifold method (Gorban et al. 2004). The Hilbert method and Chapman–Enskog method suffer from the drawback that they are only applicable to the small Knudsen number cases. The invariant manifold method and its results are too complicated for engineering applications. Although the Grad method is quite successful for describing the second sound effect in massive fluids at low temperature in particular, the situations slightly deviating from the classical Navier–Stokes–Fourier domain in general, it failed to work in cases with sharp time–space dependence such as the strong shock wave. In the present work, we attempt to propose a coarse-graining approach and derive a ballistic-diffusive heat conduction model from the BTE.

2. Boltzmann transport equation

Under the assumption that no external force exerts on the system, the BTE reads

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = Q(f, f),$$

where $f(r, \varepsilon, t)$ is the distribution function which describes the probability of finding a particle with the kinetic energy $\varepsilon$ near the point $r$ at time $t$, $Q(f, f)$ is the nonlinear Boltzmann collision integral. In order to simplify equation (2.1), several kinetic models have been developed. Among them, the most well-known is the Bhatnagar–Gross–Krook model (Bhatnagar et al. 1954)

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = -\frac{f - f_0}{\tau},$$

where $f_0$ is the equilibrium distribution function, $\mathbf{v}$ is the velocity of heat carrier, $\tau$ is the relaxation time that is approximated by the Mathiessen rule

$$\frac{1}{\tau} = \frac{1}{\tau_u} + \frac{1}{\tau_i} + \frac{1}{\tau_b},$$

where $\tau_u$, $\tau_i$ and $\tau_b$ are the mean free times related to Umklapp processes, collision with impurities and boundary scattering, respectively.

Equation (2.2) can be approximated by the following equation (Cheng et al. 2008):

$$\frac{f(r, \varepsilon, t + \Delta t) - f(r, \varepsilon, t)}{\Delta t} + \mathbf{v} \cdot \nabla f(r, \varepsilon, t) = -\frac{f(r, \varepsilon, t) - f_0(r, \mathbf{v})}{\tau}. \quad (2.3)$$

Setting $\Delta t = \tau$, equation (2.3) becomes

$$\tau \mathbf{v} \cdot \nabla f(r, \varepsilon, t) + f(r, \varepsilon, t + \tau) = f_0. \quad (2.4)$$

With the help of the distribution function $f$, the heat flux vector $\mathbf{q}(r, t)$ is expressed as follows (Xu & Wang 2005):

$$\mathbf{q}(r, t) = \int_\varepsilon \mathbf{v}(r, t)f(r, \varepsilon, t)\varepsilon D(\varepsilon) \, d\varepsilon, \quad (2.5)$$

where $D(\varepsilon)$ is the density of states.

### 3. From Boltzmann transport equation to heat conduction model

We start with deriving the classical Fourier law from the BTE (Tien et al. 1998). Assume that the distribution function $f$ is independent of the time $t$, and $\nabla f \approx \nabla f_0$, then equation (2.2) becomes

$$f = f_0 - \tau \mathbf{v} \cdot \nabla f_0, \quad (3.1)$$

which is called the quasi-equilibrium approximation. Since the equilibrium distribution function $f_0$ is dependent on the temperature, we have

$$\nabla f_0 = \frac{df_0}{dT} \nabla T. \quad (3.2)$$

Equations (3.1) and (3.2) enable us to rewrite equation (2.5) as follows:

$$\mathbf{q}(r, t) = \int_\varepsilon \mathbf{v}f_0\varepsilon D(\varepsilon) \, d\varepsilon - \int_\varepsilon \tau \mathbf{vv} \frac{df_0}{dT} \varepsilon D(\varepsilon) \, d\varepsilon \cdot \nabla T. \quad (3.3)$$

The first term containing $f_0$ on the right-hand side of this equation drops out as the integral over all the directions becomes zero. Therefore,

$$\mathbf{q}(r, t) = -\lambda_0 \cdot \nabla T, \quad (3.4)$$

with

$$\lambda_0 = \int_\varepsilon \tau \mathbf{vv} \frac{df_0}{dT} \varepsilon D(\varepsilon) \, d\varepsilon. \quad (3.5)$$
If the heat conduction medium is isotropic, equation (3.4) reduces to

\[ q(r, t) = -\lambda_0 \nabla T, \]  

(3.6)

where \( \lambda_0 \) is the thermal conductivity. Equation (3.6) is nothing more than the classical Fourier law of heat conduction.

From the approximate BTE (2.4), a similar derivation process to that above gives rise to the single-phase-lagging heat conduction model (Cheng et al. 2008)

\[ q(r, t + \tau) = -\lambda_0 \nabla T(r, t). \]  

(3.7)

Notice that the quasi-equilibrium assumption has been made in order to re-derive the Fourier law from the BTE. However, for many nanoscale heat conduction problems, the characteristic length of the system is comparable or smaller than the mean free path of heat carriers, thus the quasi-equilibrium assumption is not valid, namely, the first-order approximation given by equation (3.1) is not enough. Contribution from higher order moments should be accounted for. In order to do this, we first try to seek some clues by recalling the Grad moment method. For this method, the following assumptions are made:

— During the time of order \( \tau \), a set of lower order moments denoted as \( M' \) does not change significantly in comparison with the rest of the higher order moments \( M'' \).

— Towards the end of the fast evolution, the values of the moments \( M'' \) are determined by the lower order moments \( M' \).

— On the time of order \( t \gg \tau \), dynamics of the distribution function are described by the dynamics of the lower order moments \( M' \).

These assumptions suggest that the distribution function \( f \) can be approximated by the following expansion in terms of the Hermite velocity tensors (Gorban et al. 2004):

\[ f^N = f_0 \left( 1 + \sum_{(a)}^N a_{(a)}(M')H_{(a)}(v - u) \right), \]  

(3.8)

where \( H_{(a)} \) are Hermite tensor polynomials and orthogonal with the weight \( f_0 \), the coefficient \( a_{(a)}(M') \) are functions of the lower order moments \( M' \), \( N \) is the highest order of \( M' \), \( u \) is the mean velocity. The evolution equations of the lower order moments \( M' \) are established by substituting equation (3.8) into the BTE. The most well-known solution obtained by this method is Grad’s 13-moment approximation, where the set of lower order moments consists of five hydrodynamic moments, five components of the traceless stress tensor and the three components of the heat flux vector.

In the following, based on the first assumption for the Grad method, we try to propose a coarse-graining approach and establish a non-Fourier heat conduction model. We first split the distribution function \( f \) into two parts:

\[ f = f_0 + f_1, \]  

(3.9)
where $f_1$ accounts for the non-equilibrium effect. Substituting equation (3.9) into equation (2.4) gives
\[ \tau v \cdot \nabla (f_0(r, \varepsilon, t) + f_1(r, \varepsilon, t)) + f_0(r, \varepsilon, t + \tau) + f_1(r, \varepsilon, t + \tau) = f_0(r, \varepsilon, t). \] (3.10)

In view of equation (2.5), multiplying $\varepsilon D(\varepsilon) v$ on both sides of equation (3.10) and integrating the resulting equation with respect to $\varepsilon$, yield
\[ \int_{\varepsilon} \tau vv \cdot \nabla (f_0(r, \varepsilon, t) + f_1(r, \varepsilon, t)) \varepsilon D(\varepsilon) \, d\varepsilon + \int_{\varepsilon} v f_1(r, \varepsilon, t + \tau) \varepsilon D(\varepsilon) \, d\varepsilon = 0. \] (3.11)

In deriving equation (3.11), the relation, $\int v f_0 \varepsilon D(\varepsilon) \, d\varepsilon = 0$ has been used. The second integral on the left-hand side of equation (3.11) is denoted as
\[ J^{(1)}(r, t + \tau) = \int_{\varepsilon} v f_1(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon. \]

Note that $q(r, t) = J^{(1)}(r, t)$. Equation (3.11) can be rewritten as
\[ J^{(1)}(r, t + \tau) = - \int_{\varepsilon} \tau vv \cdot \nabla f_0(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon - \int_{\varepsilon} \tau vv \cdot \nabla f_1(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon. \] (3.12)

The same manipulation as the derivation of the Fourier law from the BTE yields
\[ J^{(1)}(r, t + \tau) = -\lambda_0 \nabla T - \int_{\varepsilon} \tau vv \cdot \nabla f_1(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon. \] (3.13)

In order to get equation (3.13), the assumption that the heat conduction medium is isotropic has been applied. Now denote $e$ as the unit vector of $v$ and assume that $\tau$ is independent of $\varepsilon$, we have
\[ J^{(1)}(r, t + \tau) = -\lambda_0 \nabla T - \tau v_1 \int_{\varepsilon} e v \cdot \nabla f_1(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon, \] (3.14)

where $v_1$ has the dimension of velocity and makes the difference between $\int_{\varepsilon} \tau vv \cdot \nabla f_1(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon$ and $\tau v_1 \int_{\varepsilon} e v \cdot \nabla f_1(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon$ as small as possible. If we only focus on the heat conduction occurring in a solid medium, then the gradient operator in the second term on the right-hand side of equation (3.14) may be put out of the integrand, that is
\[ J^{(1)}(r, t + \tau) = -\lambda_0 \nabla T - \tau v_1 \nabla \cdot \int_{\varepsilon} e v f_1(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon. \] (3.15)

Introducing the following notation:
\[ J^{(2)}(r, t) = - \int_{\varepsilon} e v f_1(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon, \] (3.16)

where $J^{(2)}$ is called the flux of the heat flux $J^{(1)}$, equation (3.15) becomes
\[ J^{(1)}(r, t + \tau) = -\lambda_0 \nabla T + \tau v_1 \nabla \cdot J^{(2)}(r, t). \] (3.17)

Multiplying $-e v e D(\varepsilon)$ on both sides of equation (3.10) yields
\[ J^{(2)}(t + \tau) - \int e v f_0(r, \varepsilon, t + \tau) \varepsilon D(\varepsilon) \, d\varepsilon = \int \tau vv \cdot \nabla f(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon. \] (3.18)
Since
\[ \int v_i v_j f_0 \varepsilon D(\varepsilon) \, d\varepsilon = \frac{5}{2} \frac{k_B^2 T^2}{m} \delta_{ij} \ll 1, \]
where \( v_i \) is the \( i \)-th component of the velocity vector \( v \), \( k_B \) is the Boltzmann constant, \( m \) is the mass of heat carrier, we have
\[ \int e v f_0(\mathbf{r}, \varepsilon, t + \tau) \varepsilon D(\varepsilon) \, d\varepsilon \ll 1. \]
Thus by neglecting this integral in equation (3.18), we have
\[ J^{(2)}(t + \tau) = \int \tau e v v \cdot \nabla f(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon. \tag{3.19} \]
Now we split \( f \) into two parts
\[ f = f_{2,0} + f_{2,1}, \tag{3.20} \]
where \( f_{2,0} \) and \( f_{2,1} \) are related to the lower and higher order moments, respectively. Substituting equation (3.20) into equation (3.19) yields
\[ J^{(2)}(t + \tau) = \int \tau e v v \cdot \nabla f_{2,0}(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon + \int \tau e v v \cdot \nabla f_{2,1}(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon. \tag{3.21} \]
Since \( v \cdot \nabla f_{2,0} = v e \cdot \nabla f_{2,0} \), here \( v \) is the magnitude of the velocity \( v \), equation (3.21) becomes
\[ \int \tau e v v \cdot \nabla f_{2,0}(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon \approx \tau \bar{v}_{2,0} \int e e v v \cdot \nabla f_{2,0}(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon, \tag{3.22} \]
where \( \bar{v}_{2,0} \) has the dimension of \( v \) and makes the difference between the two terms on both sides of equation (3.22) as small as possible. The gradient of \( f_{2,0} \) can be expressed as follows:
\[ \nabla f_{2,0} = ee \cdot \nabla f_{2,0} + e^\perp e^\perp \cdot \nabla f_{2,0} + e^\perp e^\perp \cdot \nabla f_{2,0}, \]
where \( e, e^\perp \) and \( e^\perp \) constitute an orthogonal basis for the three-dimensional velocity space. In comparison with \( f_{2,1}, f_{2,0} \) involves the lower order moments. In accordance with the first assumption for the Grad method, the term \( e \cdot \nabla f_{2,0} \) does not experience the significant change with the variation of the direction of the velocity \( v \). Therefore,
\[ ee \cdot \nabla f_{2,0} \approx \frac{1}{3} \nabla f_{2,0}. \]
This allows us to rewrite equation (3.22) in the following form:
\[ \int \tau e v v \cdot \nabla f_{2,0}(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon \approx \tau v_{2,0} \int \nabla f_{2,0}(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon, \tag{3.23} \]
where \( v_{2,0} = (1/3) \bar{v}_{2,0} \). While the second term on the right-hand side of equation (3.21) can be written as
\[ \int \tau e v v \cdot \nabla f_{2,1}(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon \approx \tau v_{2,1} \int e e v v \cdot \nabla f_{2,1}(r, \varepsilon, t) \varepsilon D(\varepsilon) \, d\varepsilon, \tag{3.24} \]
where $v_{2,1}$ has the dimension of velocity and makes the difference between the terms on both sides of equation (3.24) as small as possible. Substituting equations (3.23) and (3.24) into equation (3.21) yields

$$J^{(2)}(t + \tau) = \tau v_{2,0} \int \nabla f_{2,0}(r, \varepsilon, t) \psi \hat{D}(\varepsilon) \, d\varepsilon + \tau v_{2,1} \int \mathbf{e} \mathbf{v} \cdot \nabla f_{2,1}(r, \varepsilon, t) \varepsilon \hat{D}(\varepsilon) \, d\varepsilon.$$ (3.25)

For the heat conduction in the solid medium, the gradient operator may be put out of the integrands in equation (3.25), so that

$$J^{(2)}(t + \tau) = \tau v_{2,0} \nabla \int v_{f_{2,0}}(r, \varepsilon, t) \varepsilon \hat{D}(\varepsilon) \, d\varepsilon + \tau v_{2,1} \int \mathbf{e} \mathbf{v} \cdot \nabla f_{2,1}(r, \varepsilon, t) \varepsilon \hat{D}(\varepsilon) \, d\varepsilon.$$ (3.26)

Since $f_{2,0}$ is related to the lower order moments, it dominates $f_1$, therefore, $\int v_{f_{2,0}}(r, \varepsilon, t) \varepsilon \hat{D}(\varepsilon) \, d\varepsilon \approx J^{(1)}(r, t)$. Thus, equation (3.26) becomes

$$J^{(2)}(t + \tau) = \tau v_{2,0} \nabla J^{(1)}(r, t) + \tau v_{2,1} \nabla \cdot J^{(3)}(r, t),$$ (3.27)

where $J^{(3)}(r, t) = \int \mathbf{e} \mathbf{v} f_{2,1}(r, \varepsilon, t) \varepsilon \hat{D}(\varepsilon) \, d\varepsilon$, which is the flux of $J^{(2)}(r, t)$. Generally, we have

$$J^{(n)}(t + \tau) = \tau v_{n,0} \nabla J^{(n-1)}(t) + \tau v_{n,1} \nabla \cdot J^{(n+1)}(t), \quad (n = 2, 3, \ldots).$$ (3.28)

The first-order Taylor expansion of $J^{(n)}(t + \tau)$ with respect to the time $t$ gives rise to

$$\tau \dot{J}^{(n)}(t) = -J^{(n)}(t) + \tau v_{n,0} \nabla J^{(n-1)}(t) + \tau v_{n,1} \nabla \cdot J^{(n+1)}(t), \quad (n = 2, 3, \ldots),$$ (3.29)

which has been obtained by Alvarez & Jou (2007) from the extended irreversible thermodynamics.

Equations (3.17) and (3.28) describe a new type of non-Fourier heat conduction model. Note that when deriving this model, we only use the first assumption for the Grad method, and have not expanded the distribution function into an orthogonal series, thus this coarse-graining approach is quite different from the Grad method.

Equations (3.17) and (3.28) consist of an infinite number of partial differential equations. For engineering applications, the simplification process is desirable.

### 4. The simplified heat conduction model

The heat conduction model established in the last section reads

$$J^{(1)}(t + \tau) = -\lambda_0 \nabla T + \tau v_1 \nabla \cdot J^{(2)}(t)$$ (4.1)

and

$$J^{(n)}(t + \tau) = \tau v_{n,0} \nabla J^{(n-1)}(t) + \tau v_{n,1} \nabla \cdot J^{(n+1)}(t), \quad (n = 2, 3, \ldots).$$ (4.2)

The application of the Fourier transformation on these equations yields

$$\tilde{J}^{(1)}(\omega, k) = -ik\lambda(\omega, k) \tilde{T}(\omega, k),$$ (4.3)
where $\omega$ is the frequency, $k$ is the wave number, $\tilde{J}^{(1)}(\omega, k)$ and $\tilde{T}(\omega, k)$ are the Fourier transforms of $J^{(1)} \equiv q$ and $T$, respectively, $\lambda(\omega, k)$ is

$$\lambda(\omega, k) = \frac{\lambda_0}{e^{i\omega t} + k^2 l_1^2/(e^{i\omega t} + (k^2 l_2^2/e^{i\omega t} + \cdots))},$$

(4.4)

where $l_1^2 = \tau^2 v_1 v_2$, $l_n^2 = \tau^2 v_{n,1} v_{n+1,0} (n = 2, 3, \ldots)$. It is worthwhile to mention that Hess (1977) derived a continued-fraction expansion analogous to equation (4.4) for mass transport from the linearized BTE. If $l_1 = l_2 = \cdots = l_n = \cdots = l/2$, equation (4.4) becomes

$$A = \frac{1}{e^{i\omega t} + (k^2 l^2/4)A},$$

(4.5)

where $A = \lambda/\lambda_0$. Solving equation (4.5) gives

$$\lambda(\omega, k) = \frac{-e^{i\omega t} + \sqrt{e^{2i\omega t} + k^2 l^2}}{k^2 l^2/2} \lambda_0.$$

(4.6)

Setting $k = 2\pi/L$ ($L$ is the size of the heat conduction medium) and $\omega = 1/\tau$, we have

$$\lambda(\omega, L) = \frac{\lambda_0}{2\pi^2 Kn^2} \left[ -e^i + \sqrt{e^{2i} + 4\pi^2 Kn^2} \right].$$

(4.7)

While the effective heat conductivity obtained by the extended irreversible thermodynamics is (Alvarez & Jou 2007)

$$\lambda'(\omega, L) = \frac{\lambda_0}{2\pi^2 Kn^2} \left[ -(1 + i) + \sqrt{(1 + i)^2 + 4\pi^2 Kn^2} \right].$$

(4.8)

For the steady case, $\omega = 0$, equation (4.6) reduces to

$$\lambda(L) = \frac{\lambda_0 L^2}{2\pi^2 l^2} \left[ \sqrt{1 + 4\left(\frac{\pi l}{L}\right)^2} - 1 \right].$$

(4.9)

By the definition of the Knudsen number, $Kn = l/L$, equation (4.9) is rewritten as follows:

$$\lambda(L) = \frac{\lambda_0}{2\pi^2 Kn^2} \left[ \sqrt{1 + 4(\pi Kn)^2} - 1 \right],$$

(4.10)

which has already been obtained by Alvarez & Jou (2007). Note that if $Kn \to 0$, then $\lambda(L) \to \lambda_0$, thus the Fourier law is recovered; if $Kn \to \infty$, then $\lambda(L) \to (\lambda_0/\pi) L/l$ which describes the ballistic heat conduction.

The real part of $\lambda(\omega, L)$ expressed by equation (4.7) is taken as the effective thermal conductivity. The size dependence of this effective thermal conductivity, the associated theoretical results given by Alvarez & Jou (2007, 2008) and experimental results obtained by Asheghi et al. (2002), Ju & Goodson (1999), Liu & Asheghi (2004) and Li et al. (2003), for silicon thin films and nanowires, are illustrated in figure 1 where the horizontal axis is for the logarithm of the effective length to base 10, the vertical axis for the effective thermal conductivity. From figure 1, one can see that the effective thermal conductivity obtained by the present work shows an agreement with the theoretical and experimental results for the silicon thin film and nanowires in the nanoscale regime.
Now the method developed by Jou et al. (1999) is employed to get the effective relaxation time, which reflects the memory effect. By the energy conservation equation

\[ \rho c_v \dot{T} = -\nabla \cdot \mathbf{q}, \] (4.11)

where \( \rho \) is the density, \( c_v \) is the specific heat at constant volume, one obtains the following dispersion relation between \( \omega \) and \( k \):

\[ i\omega = -\chi k^2 e^{i\omega \tau} \pm \sqrt{e^{i2\omega \tau} + k^2 l^2 / k^2 l^2 / 2}, \] (4.12)

where \( \chi \) is the thermal diffusivity. Thus the phase velocity \( \nu_p = \omega / Re(k) \) satisfies

\[ \frac{\nu_p^4}{\omega^2} \cos^2 \omega \tau + \left( -l^2 + \frac{4\chi \sin \omega \tau}{\omega} \right) \nu_p^2 - 4\chi^2 = 0. \] (4.13)

When \( \omega \) is large enough, we have

\[ \left( -l^2 + \frac{4\chi \sin \omega \tau}{\omega} \right) \nu_p^2 - 4\chi^2 = 0, \]

that is

\[ \nu_p^4 = \frac{\chi}{(\sin \omega \tau / \omega)-(l^2 / 4\chi)}. \] (4.14)
Setting $\omega = 1/\tau$, equation (4.14) becomes

$$
\nu_b^2 = \frac{\chi}{\tau \sin(1.0) - (l^2/4\chi)}.
$$

(4.15)

Thus, we may introduce the effective relaxation time $\tau_e$ in the following way:

$$
\tau_e = \tau \sin(1.0) - \frac{l^2}{4\chi}.
$$

(4.16)

By equations (4.9) and (4.16) as well as the single-phase-lagging heat conduction model (3.7), the following non-Fourier heat conduction model is obtained:

$$
q(r, t + \tau_e) = -\lambda(L)\nabla T(r, t).
$$

(4.17)

In this model, both the memory and size effects are accounted for by the lagging time $\tau_e$ and the dependence of the effective heat conductivity $\lambda(L)$ on the size of the heat conduction medium.

Now we show that the model (4.17) is Galilean invariant. Under the following Galilean transformation:

$$
\mathbf{r}' = \mathbf{r} - U t, \quad t = t, \quad T'(\mathbf{r}', t) = T(\mathbf{r}', t) \quad \text{and} \quad q'(\mathbf{r}', t) = q(\mathbf{r}, t),
$$

equation (4.17) becomes

$$
q'(\mathbf{r}', t + \tau_e) = -\lambda(L)\nabla_{\mathbf{r}'} T'(\mathbf{r}', t),
$$

(4.18)

where $\nabla_{\mathbf{r}'}$ represents the gradient operator acting on the variable $\mathbf{r}'$. From equation (4.18), it is evident that the ballistic-diffusive heat conduction model (4.17) satisfies the Galileo’s principle of relativity.

5. A one-dimensional heat conduction problem

As mentioned in §1, Chen (2001, 2002) has derived a new type of heat conduction equations, called the ballistic-diffusive equations, from the BTE. The main point of this method is to artificially split the distribution function into two parts, $f = f_b + f_m$, where $f_b$ originates from the boundary of heat conduction medium and represents the contribution from the ballistic heat conduction, $f_m$ originates from inside the domain and reflects the contribution from the diffusive heat conduction. Subsequently, the temperature $T$ and the heat flux $q$ are also divided into two parts $T_b$, $T_m$ and $q_b$, $q_m$, respectively. $f_b$ and $f_m$ satisfy the BTE without the nonlinear collision term and the approximate BTE under the relaxation time approximation, respectively. Based on these two equations, Chen (2001) established the ballistic-diffusive equations. However, this approach suffers from a drawback that it can not give the anticipated uniform internal energy at equilibrium. Furthermore, as pointed in Jou et al. (2010), the ballistic-diffusive equations assume the following constitutive relations:

$$
\tau \frac{\partial q_b}{\partial t} + q_b = -k \nabla T_b \quad \text{and} \quad \tau \frac{\partial q_m}{\partial t} + q_m = -k \nabla T_m,
$$

where $k$ is the bulk heat conductivity of the material under consideration. These constitutive relations are nothing more than the Maxwell–Cattaneo law, which can not describe the size effect occurring in the nanoscale heat conduction. Furthermore, the Maxwell–Cattaneo violates the second law of thermodynamics (Christov & Jordan 2005). The impact of the ballistic heat conduction or the size effect is reflected by a term $\nabla \cdot \mathbf{q}_b$ in the ballistic-diffusive equations. While in the model (4.17) the ballistic heat transport is described by the dependence of the heat conductivity on the Knudsen number.

In this section, we apply the heat conduction model (4.17) to a one-dimensional nanoscale heat conduction problem that has been discussed by Chen (2001, 2002). The results obtained will be compared with the solutions of the ballistic-diffusive equations and the Fourier heat conduction equation.

Combining equations (4.11) and (4.17), we obtain the following heat conduction equation:

$$
\frac{\partial T(r, t + \tau_e)}{\partial t} = \frac{\lambda(L)}{\rho c_v} \Delta T(r, t). 
$$  \hspace{1cm} (5.1)

The first-order Taylor expansion of the term on the left-hand side of equation (5.1) leads to

$$
\frac{\partial T(r, t)}{\partial t} + \tau_e \frac{\partial^2 T(r, t)}{\partial t^2} = \frac{\lambda(L)}{\rho c_v} \Delta T(r, t). 
$$  \hspace{1cm} (5.2)

Now we consider a transient heat conduction problem of thin films: at the initial time, $T(x, t)|_{t=0} = 0.0$, at $t = 0^+$ one suddenly imposes $T(0, t) = 1.0$ at one surface of the thin film, and keeps $T(1, t)| = 0.0$ at the opposite surface. This heat conduction problem has been discussed by Chen (2001, 2002) based on the ballistic-diffusive equations. By equation (5.2), this problem can be mathematically formulated as follows:

$$
\begin{align*}
\frac{\partial T(x, t)}{\partial t} + \tau_e \frac{\partial^2 T(x, t)}{\partial t^2} &= \frac{\lambda(L)}{\rho c_v} \frac{\partial^2 T(x, t)}{\partial x^2}, \\
T(x, t)|_{t=0} &= 0, \quad \left. \frac{\partial T(x, t)}{\partial t} \right|_{t=0} = 0 \quad \text{and} \quad T(0, t) = 1.0, T(1.0, t) = 0.
\end{align*} \hspace{1cm} (5.3)
$$

Define the following non-dimensional parameters:

$$
t^* = \frac{t}{\tau} \quad \text{and} \quad x^* = \frac{x}{L},
$$

where $L = 1.0$, and use the relation $\lambda_0 = (1/3) Cv_l$ ($v$ is velocity of heat carrier), here $C = \rho c_v$, we have

$$
\begin{align*}
\frac{\partial T(x^*, t^*)}{\partial t^*} + c_0 \frac{\partial T^2(x^*, t^*)}{\partial t^{*2}} &= \lambda \frac{\partial^2 T(x^*, t^*)}{\partial x^{*2}}, \\
T(x^*, t^*)|_{t^*=0} &= 0, \quad \left. \frac{\partial T(x^*, t^*)}{\partial t^*} \right|_{t^*=0} = 0 \quad \text{and} \quad T(0, t^*) = 1.0, T(1.0, t^*) = 0.
\end{align*} \hspace{1cm} (5.4)
$$
where \( c_0 = \sin(1.0) - 0.75, \lambda = (1/6\pi)(\sqrt{1 + 4\pi^2Kn^2} - 1) \). Solving this initial-boundary problem yields

\[
T(x^*, t^*) = \sum_{j=1}^{\infty} \frac{1}{j\pi} \frac{1}{c_0^2} e^{-\frac{1}{2c_0^2} t^*} \left[ -2\cos(c_j t^*) - \frac{1}{c_0 c_j} \sin(c_j t^*) \right] \sin(j\pi x^*) - x^* + 1, \tag{5.5}
\]

where \( c_j = (1/2c_0)\sqrt{4c_0^2\pi^2\lambda - 1} \).

From equation (5.5), the non-dimensional heat flux at the boundary \( x^* = 0 \) is expressed as

\[
q^*|_{x^*=0} = \frac{q}{Cv \Delta T} \bigg|_{x^*=0} = \frac{1}{6\pi^2Kn} \left( \sqrt{1 + 4\pi^2Kn^2} - 1 \right) - \frac{1}{6c_0^2\pi^2Kn} \left( \sqrt{1 + 4\pi^2Kn^2} - 1 \right)
\times \sum_{j=1}^{\infty} \frac{e^{-(t^*/2c_0)}}{1 + 4c_0^2c_j^2} \left( -8c_0^2 c_j - \frac{2}{c_j} \right) \sin(c_j t^*), \tag{5.6}
\]

where \( \Delta T = 1.0 \). Note that in order to compare with the results obtained by Chen (2001, 2002) the same normalization procedure for the heat flux has been applied. The variations of \( q^*|_{x^*=0} \) with respect to the time which are obtained from equation (5.6), the ballistic-diffusive equations (Chen 2001, 2002) and the Fourier law, are displayed in figure 2 (the horizontal axis is for the logarithm of time to base 10) for the case \( Kn = 10.0 \). One can see that the non-dimensional heat flux at the boundary \( x^* = 0 \) expressed by equation (5.6) is lower than the result obtained by the classical heat conduction equation, which agrees with the experimental observation (Larson et al. 1986). In comparison with the result obtained by Chen (2001, 2002), our result is larger at earlier time and smaller at later time. The discrepancy may be caused by the different boundary conditions as well as the different definitions of the temperature between our model and Chen’s model.
6. Concluding remarks

A coarse-graining method for the reduced description of the BTE is developed and applied to the heat conduction modelling. The obtained non-Fourier heat conduction model can be viewed as the extension of the single-phase-lagging heat conduction model, and thus it takes into account of the memory effect and avoids the infinite heat propagation speed. Furthermore, the thermal conductivity in this model depends on the Knudsen number, when the Knudsen number tends to zero or infinity, the heat conduction model reduces to the single-phase-lagging heat conduction model or the ballistic heat conduction model, respectively. Therefore, the non-Fourier heat conduction model developed in this work may cover the ballistic to diffusive regimes of heat conduction. The comparison of the dependence of the effective thermal conductivity on the size of the heat conduction medium with the available theoretical and experimental results shows an agreement for silicon thin films and nanowires in the nanoscale regime. Finally, we prove that the proposed model is Galilean invariant.

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