Ballistic-Diffusive Heat-Conduction Equations

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We present new heat-conduction equations, named ballistic-diffusive equations, which are derived from the Boltzmann equation. We show that the new equations are a better approximation than the Fourier law and the Cattaneo equation for heat conduction at the scales when the device characteristic length, such as film thickness, is comparable to the heat-carrier mean free path and/or the characteristic time, such as laser-pulse width, is comparable to the heat-carrier relaxation time.

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It is well known that the diffusion heat conduction equation based on the Fourier law, $q = -k\partial T/\partial x$, leads to the unreasonable result that heat propagates at an infinite speed. To resolve this dilemma, the Cattaneo equation, $\tau\partial q/\partial t + q = -k\partial T/\partial x$, was proposed [1]. This leads to a wave type of heat conduction equation called the telegraph equation or hyperbolic heat-conduction equation (see Ref. [2] for a comprehensive review). A mechanism that is not included in the hyperbolic equation is the ballistic transport, which becomes important when the sample size is smaller than the mean free path or the temperature gradient becomes large. A nonlocal heat-conduction model was developed by Mahan and Claro based on the steady-state Boltzmann equation [3]. The model, however, does not include the retardation of heat carriers (electrons, phonons, or molecules) due to their finite speed of propagation. Joshi and Majumdar [4] compared the solutions of the transient Boltzmann equation, the Fourier law, and the Cattaneo equation for phonon heat conduction perpendicular to a thin film plane. They concluded that neither the Fourier nor the Cattaneo equation can represent well the heat-conduction processes in small scale and/or fast transient. The Boltzmann equation, even in its simplest form, however, is difficult to solve because it involves variables in both real and momentum spaces, as well as time. In this article, we establish the ballistic-diffusive heat-conduction equations and demonstrate that they are a good approximation of the transient Boltzmann equation. Its advantage over the Boltzmann equation is that only spatial coordinates and time are involved. Unlike the Fourier law and the Cattaneo equation, the new set of equations capture both the time retardation and the nonlocal transport process, and thus can be applied to fast heat-conduction processes and to small structures. Yet these equations are simple enough that the existing numerical tools can be readily applied for complicated heat-conduction problems in small structures, as long as the particle description is still valid.

Similar to previous treatments [3–5], our starting point is the Boltzmann equation under the relaxation time approximation,

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f = -\frac{f - f_0}{\tau(\omega)}, \quad (1)$$

where f is the carrier distribution function, f_0 is the equilibrium distribution, $\mathbf{v}$ is the carrier group velocity, and τ is the heat-carrier relaxation time which usually depends on the angular frequency ω (or energy) of the heat carriers. In theory, the relaxation time may also depend on the wave vector (direction). In heat conduction, most theoretical treatment is based on isotropic scattering such that consideration of the frequency dependence is sufficient.

The essence of the ballistic-diffusive approximation is to divide the distribution function at any point into two parts, $f = f_b + f_m$, as shown in Fig. 1. In this figure, f_b at an internal point along a specific direction originates from the boundaries. In the course of traveling from the boundary

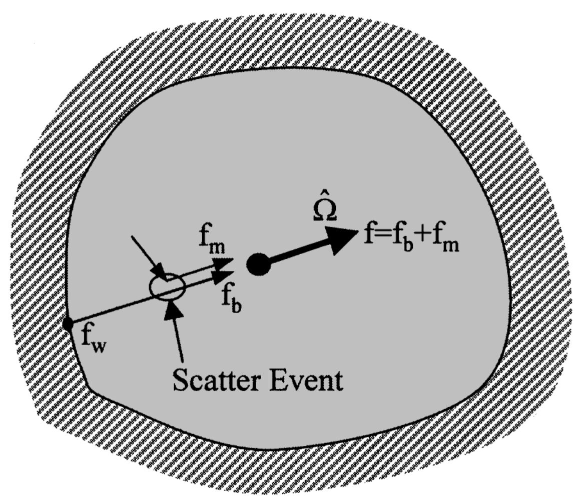

FIG. 1. In deriving the ballistic-diffusive heat-conduction equations, local carrier distribution function f is divided into two parts: f_b originates from the boundary (f_w) and experiences outgoing scattering only, and f_m originates from inside the domain and is directed into the $\hat{\Omega}$ direction either through scattering or through emission of the medium.

to this point, some of the carriers are scattered and only those remaining are included in f_b. This part of carriers is ballistic. The rest of the carriers at this internal point is grouped into f_m. These are the carriers that are scattered or emitted into this direction from other internal points. The distribution of these carriers is more isotropic than the ballistic carriers from the boundary due to multiple scattering or nearly isotropic emission. The philosophy is then to treat this part of the heat carriers by the conventional diffusion approach, as will be derived from the spherical harmonic expansion of the distribution function f_m. Such an approach was successfully used for steady-state photon transport [6,7]. With such a division of the local carrier constitutions, the local heat flux and temperature are also made of two parts, as will be given later. For the ballistic part, we have

$$\frac{1}{|\mathbf{v}|}\frac{\partial f_b}{\partial t} + \hat{\Omega}\cdot\nabla f_b = -\frac{f_b}{|\mathbf{v}|\tau}, \qquad (2)$$

and $\hat{\Omega}$ is the unit vector in the direction of carrier propagation. A general solution for Eq. (2) is

$$f_b(t,\mathbf{r},\hat{\Omega}) = f_w[t-(s-s_0)/|\mathbf{v}|, \mathbf{r}-(s-s_0)\hat{\Omega}] \times \exp\left(-\int_{s_0}^{s}\frac{ds}{|\mathbf{v}|\tau}\right), \qquad (3)$$

where f_w is the value of the carrier distribution function at the boundary point s_0 along direction $\hat{\Omega}$; $s-s_0$ is the distance along the propagation direction. The boundary value f_w includes those reflected and also emitted carriers at the boundary. The governing equation for f_m is

$$\frac{\partial f_m}{\partial t} + \mathbf{v}\cdot\nabla f_m = -\frac{f_m - f_0}{\tau}. \qquad (4)$$

As explained, f_m includes scattered and emitted carriers from the internal region into the specific direction being considered. This part is more isotropic and will be treated by the diffusion approximation. We introduce the spherical harmonic expansion for f_m and maintain the first two terms as an approximation, which is often used in solving the Boltzmann equation for thermal radiation and neutron transport [7],

$$f_m(t,\mathbf{r},\hat{\Omega}) = g_0(t,\mathbf{r}) + \mathbf{g}_1(t,\mathbf{r})\cdot\hat{\Omega}, \qquad (5)$$

where $\mathbf{g}_1$ is a vector that is related to the heat flux, and g_0 is a scalar that represents the average of f_m over all propagation directions. The latter is related to the local internal energy u_m and temperature T_m due to the diffusive part of the carriers. Substituting Eq. (5) into Eq. (4), multiplying the obtained equation by $\hat{\Omega}$ and integrating over the solid angle of the whole space lead to [7]

$$\frac{1}{|\mathbf{v}|}\frac{\partial \mathbf{g}_1}{\partial t} + \nabla g_0 = -\frac{\mathbf{g}_1}{\Lambda}, \qquad (6)$$

where $\Lambda = |v|\tau$ is the mean free path. From the distribution function, we can calculate the heat flux and the internal energy as

$$\mathbf{q}(t,\mathbf{r}) = \frac{1}{4\pi}\int \mathbf{v}\hbar\omega(f_b + f_m)\,d^3\mathbf{v} = \mathbf{q}_b(t,\mathbf{r}) + \mathbf{q}_m(t,\mathbf{r}), \qquad (7)$$

$$u(t,\mathbf{r}) = \frac{1}{4\pi}\int \hbar\omega(f_b + f_m)\,d^3\mathbf{v} = u_b(t,\mathbf{r}) + u_m(t,\mathbf{r}), \qquad (8)$$

where $\hbar$ is the Planck constant divided by 2π and $\hbar\omega$ is the energy of each carrier. The integration is performed over the momentum space. We further introduce two temperatures T_b and T_m such that

$$\frac{\partial u}{\partial t} = C\frac{\partial T}{\partial t} = \frac{\partial u_m}{\partial t} + \frac{\partial u_b}{\partial t} = C\left(\frac{\partial T_m}{\partial t} + \frac{\partial T_b}{\partial t}\right), \qquad (9)$$

where $T = T_m + T_b$ can be considered the local temperature. It should be reminded that, in the ballistic regime, the statistical distribution of heat carriers deviates far from equilibrium such that temperature cannot be defined in the sense of equilibrium or local equilibrium. The local temperature is best considered as a measure of the local internal energy [8]. Under the current approach, the local internal energy is made of two parts: the ballistic part u_b from the boundary, and the diffusive part u_m from the internal region. Consequently, T_m and T_b are a measure of the magnitude of these two internal energy constituents, respectively.

Substituting Eq. (5) into the corresponding expression for $\mathbf{q}_m$ in Eq. (7) leads to

$$\mathbf{q}_m(t,\mathbf{r}) = \tfrac{1}{3}\int |\mathbf{v}|\hbar\omega\mathbf{g}_1 D(\omega)\,d\omega, \qquad (10)$$

where $D(\omega)$ is the density of states of carriers. In obtaining Eq. (10), we have converted the integration over momentum space into the integration over frequency through $D(\omega)$, and used the fact that the integration of $\mathbf{v}\cdot g_0$ over the whole space angle is zero because it is an odd function. The factor of $\frac{1}{3}$ in Eq. (10) is the standard kinetic factor obtained after projecting the $\mathbf{v}^2$ in the direction of heat flux.

Multiplying Eq. (6) by $\Lambda|v|\hbar\omega D(\omega)/3$ and integrating it over ω yields

$$\tau\frac{\partial \mathbf{q}_m}{\partial t} + \mathbf{q}_m = -k\nabla T_m, \qquad (11)$$

where τ is an average of the frequency dependent relaxation time and k is the thermal conductivity, $k = \int C_\omega v\Lambda\,d\omega/3 \approx Cv\Lambda/3$, C_ω is the specific heat of heat carriers at frequency ω, and C is the total specific heat. The second equation for k further assumes that the normally frequency dependent mean free path Λ can be represented by an average value. In obtaining Eq. (11), we have used the fact that $\int \nabla g_0\Lambda|v|\hbar\omega D(\omega)\,d\omega/3 = k\nabla T_m$. Equation (11) is identical to the Cattaneo equation in form. However, in the current model, $\mathbf{q}_m$ represents only part of the heat flux while, in the Cattaneo equation, it represents all the heat flux. Since the equation contains both $\mathbf{q}_m$ and T_m, we will use the energy conservation equation to eliminate $\mathbf{q}_m$:

$$-\nabla \cdot \mathbf{q} + \dot{q}_e = \frac{\partial u}{\partial t}, \tag{12}$$

where $\dot{q}_e$ is heat generation per unit volume due to external heat sources. Substituting Eqs. (7) and (9) into the above equation leads to $-\nabla \cdot \mathbf{q}_m - \nabla \cdot \mathbf{q}_b + \dot{q}_e = C(\partial T_m/\partial t + \partial T_b/\partial t)$. Eliminating $\mathbf{q}_m$ in this equation and Eq. (11), we obtain the governing equation for the diffusive component,

$$C\left(\tau \frac{\partial^2 T_m}{\partial t^2} + \frac{\partial T_m}{\partial t}\right) = \nabla(k\nabla T_m) - \nabla \cdot \mathbf{q}_b + \left(\dot{q}_e + \tau \frac{\partial \dot{q}_e}{\partial t}\right), \tag{13}$$

where we have used the following relation, $\tau C \times (\partial^2 T_b/\partial t^2) + C(\partial T_b/\partial t) = -\tau \partial(\nabla \cdot q_b)/\partial t$, that can be derived from Eq. (2) similar to the derivation of Eq. (11). The major difference of Eq. (13) compared to the hyperbolic heat-conduction equation is that an additional ballistic term $\nabla \cdot \mathbf{q}_b$ appears in the equation. These ballistic heat fluxes can be calculated from Eq. (3):

$$\mathbf{q}_b(t,\mathbf{r}) = \frac{1}{4\pi} \int \left[\int |\mathbf{v}| \hbar\omega D(\omega) f_w[t - (s - s_0)/|\mathbf{v}|, \mathbf{r} - (s - s_0)\hat{\Omega}] \exp\left(-\int_{s_0}^{s} \frac{ds}{|\mathbf{v}|\tau}\right) \cos\theta \, d\Omega \right] d\omega, \tag{14}$$

and it depends only on the T_b values at the boundaries through f_w, which can be assumed to be a known quantity when solving Eq. (13). In Eq. (14), θ is the angle formed between $\mathbf{v}$ and $\mathbf{q}$, and Ω is the solid angle in space. We will call Eqs. (13) and (14), together with the accompanying heat flux and temperature definitions, the ballistic-diffusive heat-conduction equations, or simply the ballistic-diffusive equations.

We now discuss the boundary conditions for the established equations. The formulation of the ballistic-diffusive equations implies that all the heat carriers originating from the boundaries be treated as the ballistic components. These boundary heat carriers may be emitted/transmitted from another medium or reflected from the same medium. Since the boundary does not contribute to the diffusive component, the diffusive heat flux at the boundary is

$$\mathbf{q}_m \cdot \mathbf{n} = -\int_{\hat{\Omega}\cdot\mathbf{n}<0} \hbar\omega(\mathbf{v} \cdot \mathbf{n}) f_m \, d^3\mathbf{v}. \tag{15}$$

Substituting Eqs. (5) and (10) into the above equation yields

$$\mathbf{q}_m \cdot \mathbf{n} = -CvT_m/2. \tag{16}$$

Substituting Eq. (16) into Eq. (11) leads to the following boundary conditions for the diffusion components:

$$\tau \frac{\partial T_m}{\partial t} + T_m = \frac{2\Lambda}{3} \nabla T_m \cdot n, \tag{17}$$

where we have used the kinetic relation $k = Cv\Lambda/3$.

As an example, we apply the ballistic-diffusive equations to transient phonon heat conduction across thin films of thickness L. The film is initially at a uniform temperature T_0. At time t, one of its surfaces is subjected to a phonon flux at a temperature T_1. Previously, Joshi and Majumdar [4] compared the Boltzmann equation, the Cattaneo equation, and the Fourier equation for the same problem and concluded that neither the Fourier nor the Cattaneo equation can be applied when the film thickness is comparable to the phonon near free path. Details of the computation will be presented in a full-length paper. We will discuss only the major results here. These results are presented in terms of the following nondimensional parameters: temperature $\theta = (T - T_0)/\Delta T$,

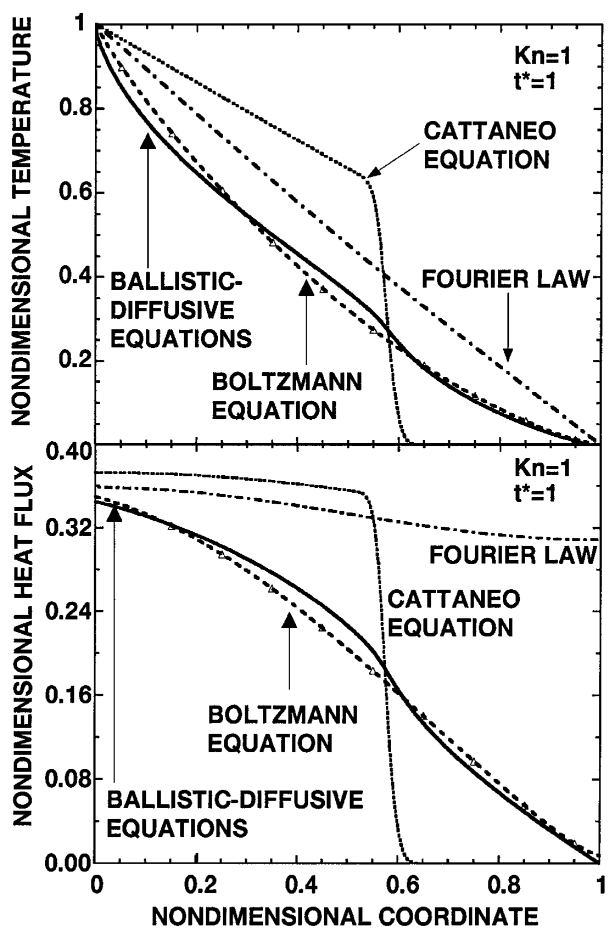

FIG. 2. Comparison of temperature and heat flux distributions obtained from the Boltzmann equation, the ballistic-diffusive equations, the Cattaneo equation, and the Fourier law for different time and phonon Knudsen number ($Kn = \Lambda/L$).

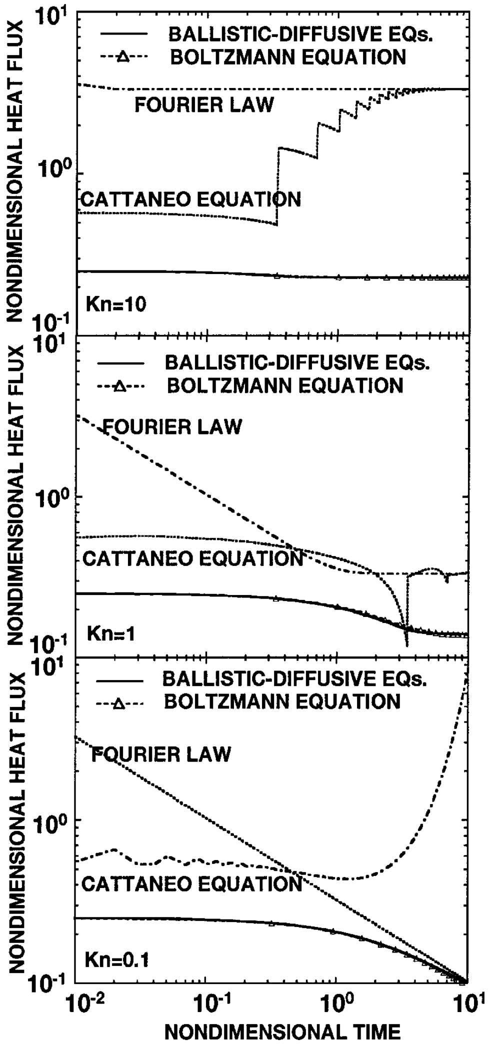

FIG. 3. Comparison of surface heat flux obtained from the Boltzmann equation, the ballistic-diffusive equations, the Cattaneo equation, and the Fourier law as a function of time for different phonon Knudsen numbers.

heat flux $q^* = q/(C\mathbf{v}\Delta T)$, time $t^* = t/\tau$, and coordinate $\eta = x/L$, where $\Delta T = T_1 - T_0$. We define the phonon Knudsen number as $Kn = \Lambda/L$. The same problem is also solved based on the Fourier heat-conduction equation, the Boltzmann equation, and the hyperbolic heat-conduction equation for comparison. Figures 2(a) and 2(b) illustrate the temperature and heat flux distributions obtained from all these approaches. Because in the ballistic-diffusive equations and in the Boltzmann equation the temperature of the incoming phonon flux is given as the boundary condition, while in the Cattaneo and the Fourier law the local equilibrium temperature is specified, we have rescaled the solution of the Boltzmann equation and the ballistic-diffusive equations based on the local temperature rather than the ΔT. Unrescaled temperature distributions would show a temperature jump at the boundaries as shown in the past work [4,9]. It clearly illustrates that the ballistic-diffusive equations are a much better approximation to the Boltzmann equation compared to the Fourier and the Cattaneo equations. Figure 3 gives the surface heat flux history based on the four different equations. The Fourier law leads to unrealistic infinite heat flux as time approaches zero and when the film thickness becomes smaller than the mean free path. The latter is consistent with the nonlocal heat-conduction model developed by Mahan and Claro [3], but the short time scale behavior cannot be predicted by that model. The Cattaneo equation creates artificial surface heat flux oscillation. The agreements between the ballistic-diffusive equation and the Boltzmann equation are excellent over a wide range of time and length scales.

In summary, we have established a new set of heat-conduction equations, named as the ballistic-diffusive heat-conduction equations, that are applicable to transient heat conduction in small structures. The equations are derived from the Boltzmann equation under the relaxation time approximation. Computational results suggest that they are a much better alternative to the Fourier and the Cattaneo equations at scales when the mean free path is comparable to the system size and when the time is comparable to the carrier relaxation time. These equations are much simpler to solve than the Boltzmann equation and can be readily incorporated into available engineering softwares to deal with fast heat-conduction processes in complicated nanostructures. We further suggest that the same methodology may be applied to deal with gas flow in microstructures and electron transport in nanoelectronic devices, in the regime where the particle description of the carriers is still valid.

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