Thin Film Phonon Heat Conduction by the Dispersion Lattice Boltzmann Method

Numerical simulations of time-dependent thermal energy transport in semiconductor thin films are performed using the lattice Boltzmann method applied to phonon transport. The discrete lattice Boltzmann Method is derived from the continuous Boltzmann transport equation assuming nonlinear, frequency-dependent phonon dispersion for acoustic and optical phonons. Results indicate that the heat conduction in silicon thin films displays a transition from diffusive to ballistic energy transport as the characteristic length of the system becomes comparable to the phonon mean free path and that the thermal energy transport process is characterized by the propagation of multiple superimposed phonon waves. The methodology is used to characterize the time-dependent temperature profiles inside films of decreasing thickness. Thickness-dependent thermal conductivity values are computed based on steady-state temperature distributions obtained from the numerical models. It is found that reducing feature size into the subcontinuum regime decreases thermal conductivity when compared to bulk values, at a higher rate than what was displayed by the Debye-based gray lattice Boltzmann method. [DOI: 10.1115/1.2944249]

Keywords: conduction, phonon, lattice Boltzmann, thermal conductivity

Introduction

The past decades have seen the development of advanced integrated circuit fabrication techniques that allow increasingly higher numbers of individual components to be built within microchips. As the characteristic lengths of individual components of electronic devices are reduced, following the trend dictated by Moore’s law, the ability to model thermal energy transport effects in those devices has turned out to be increasingly important. At such small length scales (currently in the order of tens of nanometers), the continuum media assumption breaks down, and it is therefore necessary to consider the physics of energy transport at a more fundamental level than what is done in macroscale, which basically implies taking into account the different energy carriers associated with specific materials. In crystalline semiconductor solids, materials of great interest to the microelectronics industry, the main energy carriers are phonons, which are quantized lattice vibrations. Thermal modeling of electronic devices has traditionally been based on the Fourier equation of heat conduction, which is valid only when the characteristic length of the device is larger than the phonon mean free path by at least one and desirable orders of magnitude and when the time scale of the process is much longer than the phonon relaxation time. It is now well established that a conventional analysis of heat transport based on Fourier’s equation leads to erroneous results when the mean free path of the heat carriers becomes comparable to or larger than the characteristic length of the domain of interest [1]. In addition, the Fourier equation assumes an instantaneous heat propagation, which leads to significant errors in the thermal predictions as the time scale of interest becomes comparable to or smaller than the relaxation time of the heat carriers [2]. Current transistor technology, for example, is yielding devices with channel lengths within the 90 nm technology node, and even smaller transistors (65 nm technology node) are in development phase as of 2005 [3]. It is clear from this that phonon transport in submicron semiconductor structures is likely to be within the subcontinuum regime and also that more accurate and consistent models for phonon transport are therefore needed in order to accurately model the thermal response of such devices.

For short time scales, on the order of the phonon relaxation time and length scales much larger than the phonon mean free path, the Cattaneo equation is developed from the Boltzmann transport equation (BTE). However, both the Cattaneo and Fourier equations are special limiting cases of the BTE, and as such, they either lack accuracy or require extensive computational efforts. Additionally, it is beyond their ability to simulate a multilength and multiscale phenomenon as required for a successful thermal simulation of microelectronic devices.

The BTE with the single relaxation time approximation can be used to accurately simulate energy transport in the subcontinuum regime, as long as the particle assumption for the heat carriers is valid, that is, whenever the time scale is longer than the collision time characteristic of a scattering event and when the characteristic length is larger than the phonon wavelength, \( \lambda \). However, when the characteristic length of the system is on the order of \( \lambda \), we can no longer assume a particle nature for phonons and will have to resort to performing a molecular dynamics analysis of the problem. Moreover, extensive computational effort is required to solve the BTE since it involves multiple variables descriptive for space, time, and momentum or velocity space.

Based on this, we consider the transport of thermal energy in microelectronic components a very important subject of study, for which an existing adequate theoretical background coming from the solid-state physics is available, and allows describing its fundamentals. In what follows, we will first describe the lattice Boltzmann method (LBM) applied to heat conduction in crystalline semiconductor solids, introducing the use of nonlinear phonon dispersion. Then, a discussion on thermal conductivity and phonon relaxation times will be presented. Following this, results will be presented for both thin film heat conduction and size-dependent thermal conductivity.

---

1Present address: Faculty of Applied Science and Engineering, 35 St. George Street, Room 170, Toronto, ON M5S 1A4, Canada.
Dispersion Lattice Boltzmann Method for Phonon Transport

The LBM is a discrete development of the BTE, which can be used to simulate energy transport problems within the applicability range of the BTE. Recent efforts in LBM implementation have been based on the Debye model, resulting in what has been called the gray LBM. The gray LBM [4–7] considers a linear dispersion relation, from which only a single frequency-independent phonon propagation speed can be computed. However, it is widely known that phonon dispersion relations in crystalline semiconductors are nonlinear and that different phonon polarizations exist for multicomponent crystalline structures, such as silicon. The nonlinear dispersion relations translate into frequency-dependent phonon parameters, such as propagation speed, energy density, mean free path, and relaxation time. It is, therefore, desirable to consider nonlinear dispersion in order to accurately predict phonon transport in crystalline semiconductors.

The dispersion model is an attempt to avoid simplified models and assumptions such as the Einstein, Debye, and semigray [8] models since all of them restrict the full use of the nonlinear dispersion relations in one way or another. This model considers all phonon polarizations and modes, without restricting the contributions of any of them, and allows the BTE to govern the physics of the energy transport process without simplifying assumptions. Starting with the dispersion relations, the dispersion model first discretizes the frequency spectrum by dividing it in a number of frequency bands, each one exhibiting a particular phonon propagation speed. Simultaneously, a lattice Boltzmann kinetic equation (LBKE) is solved for each discrete frequency band at each discrete time step. Total energy density is found by a proper integration of the frequency-dependent energy density, and the physics of phonon transport in each frequency band is coupled to all other bands via a common lattice temperature and an appropriate expression for the frequency-dependent relaxation times.

Phonon propagation speed, density of state, energy density, and heat capacity are computed as functions of phonon polarization and frequency. We use the dispersion relations presented by Dolling [9] for silicon in the (100) direction, which, having a diatomic crystal structure, displays both acoustic and optical, longitudinal and transverse phonon polarizations. There are two degenerate transverse modes for both acoustic and optical polarizations (denoted as TA and TO), and one longitudinal mode per phonon branch (denoted as LA and LO). The phonon propagation speed can be computed from the dispersion relations as the first derivative of phonon frequency with respect to phonon wave number [10]. From this, it was found that LA phonons propagate with the fastest speeds ranging from almost 9000 m/s to slightly above 5000 m/s. Transverse acoustic phonons are slower, but they exhibit a greater range of speeds, from about 7000 m/s to almost zero. Traditionally, optical phonons have been considered too slow to effectively contribute to thermal transport, and therefore, several approaches model them by entirely neglecting the propagation speed on the grounds that it is sufficiently close to zero (as in the Einstein, semigray, and Narumachi [11] models). However, as we have found, longitudinal optical phonons have a propagation speed ranging from 4000 m/s to almost zero, which is comparable to the propagation speed of acoustic phonons, both LA and TA. It was found that TO phonons also posses a range of propagation speeds from about 1200 m/s to almost zero, although it could be argued that these speeds are negligible when compared to the fastest propagating modes of LA phonons. It is our intent to solve simultaneous BTEs for all phonon polarization modes, which, in our view, is a more fundamental approach than those previously described. Eliminating the common assumption of zero propagation speed for optical phonons allows us to consider a more accurate physical modeling of the phonon transport process.

The phonon energy density can be computed from an adequate manipulation of the phonon dispersion relations. The energy density for a polarization \( p \) can be written as the frequency integral of Planck’s constant, phonon frequency, phonon distribution function, and phonon density of states as

\[
e_p = \int_{\Delta \omega_p} \frac{h \omega_p fD(\omega_p) \omega_p}{e^{\frac{h \omega_p}{k_B T}} - 1} \tag{1}
\]

Here, the phonon distribution function is given by the solution of the BTE with appropriate boundary conditions. Under equilibrium conditions, the phonon distribution function is given by the Bose–Einstein equilibrium distribution,

\[
f^0 = \frac{1}{e^{\frac{h \omega}{k_B T}} - 1}
\]

The total phonon energy density, which is a function of temperature, can be computed as the sum of the contributions from all phonon branches, or

\[
e_T = \sum_p e_p = e_{LA} + 2e_{TA} + e_{LO} + 2e_{TO}
\]

The next step in the setup of the dispersion model is the discretization of the frequency spectrum for all phonon branches and modes. This essentially means that the continuous dispersion relation is divided into discrete frequency bands of prescribed bandwidth \( \Delta \omega \). The total number of frequency bands for each phonon branch and mode is determined by the accuracy of the solution, in a way similar to how spatial meshes are refined until a mesh-independent solution is achieved. It is important to note that since each phonon branch and mode has a different frequency range, the discretization of each frequency spectrum will likely have different bandwidths. Once the frequency spectrum is discretized and each discrete frequency band is determined, a band-averaged phonon propagation speed is found by using

\[
r_{\Delta \omega} = \frac{1}{\Delta \omega} \int_{\Delta \omega} v(\omega) d\omega
\]

which applies to each frequency band for all phonon branches and modes. One important consequence of discretizing the frequency spectrum is that it directly affects the LBM site-to-site transport restriction. Since this restriction relates the length of the site-to-site distance (also known as lattice distance) to the magnitude of the discrete time step, or \( \Delta t = c_s \Delta x \), we observe that for different discrete propagation speeds \( c_s \) we either have different lattice spacings or different time step magnitudes. In our approach, the time step is fixed to a sufficiently small value compared to the phonon relaxation time, thus allowing acceptable temporal accuracy for all frequency bands. As a consequence, the lattice spacing for each band is different and given by the site-to-site transport restriction. Therefore, another main characteristic of the dispersion LBM is that it solves simultaneous LBKEs for each discrete frequency bands, each one having its own spatial discretization. The numerical integration necessary to find the phonon energy density at a given position within the spatial domain requires the use of an interpolation scheme every time step since the lattice sites for different discrete frequency bands do not necessarily coincide at the same location. In consequence, there will be as many different spatial discretizations as frequency bands times the number of phonon branches and modes. After performing spatial refinement studies, results are independent of frequency spectrum discretization when using 51 frequency bands for each phonon branch and mode.

Derivation of the LBKE. The LBKE for the dispersion model can be directly derived from a BTE form, under the relaxation time approximation, expressed in terms of the phonon distribution function. As mentioned, all relevant phonon parameters are frequency dependent. The derivation that follows applies to a single frequency band, but it is at the same time valid for any and all frequency...
where \( f \) is the phonon distribution function, \( f^0 \) is the equilibrium phonon distribution function, \( \nu \) the frequency-dependent phonon propagation speed, and \( \tau \) the frequency-dependent phonon relaxation time. The first derivatives of the phonon distribution function with respect to time and space can be discretized as

\[
\frac{\partial f}{\partial t} + \nu \cdot \nabla f = \frac{f^0 - f}{\tau} \tag{5}
\]

where \( f \) is the phonon distribution function, \( f^0 \) is the equilibrium phonon distribution function, \( \nu \) the frequency-dependent phonon propagation speed, and \( \tau \) the frequency-dependent phonon relaxation time. The first derivatives of the phonon distribution function with respect to time and space can be discretized as

\[
\frac{\partial f}{\partial t} = \frac{f(x,t+\Delta t) - f(x,t)}{\Delta t}
\]

\[
\frac{\partial f}{\partial x} = \frac{f(x+\Delta x,t+\Delta t) - f(x,t+\Delta t)}{\Delta x} \tag{6}
\]

Introducing the directionality subscript \( i \) in order to account for phonon propagation in a discrete lattice direction, then denoting the frequency-dependent discrete phonon propagation speed along the discrete direction \( i \) as \( c_i \), and substituting Eqs. (6) and (7) into the BTE expression given by Eq. (5), we obtain

\[
f_i(x,t+\Delta t) = f_i(x,t) + \frac{\Delta t}{\tau} \left( f_i^0(x,t) - f_i(x,t) \right) \tag{8}
\]

\[
f_i(x,t+\Delta t) - f_i(x,t) = \frac{\Delta t}{\tau} \left( f_i^0(x,t) - f_i(x,t) \right)
\]

Rearranging this equation and defining a weight factor \( W_i = \Delta t/\tau \), where \( \Delta t \) is the time step, we can write the LBKE that governs the scattering and propagation of phonons in the lattice as

\[
f_i(x+c_i\Delta x,t+\Delta t) = (1-W_i)f_i(x,t) + W_i f_i^0(x,t) \tag{9}
\]

The total phonon distribution function is the sum of discrete phonon distributions along all discrete lattice directions \( D \),

\[
f(x,t) = \sum_{i=1}^{D} f_i(x,t) \tag{10}
\]

The equilibrium phonon distribution function in this case is computed directly from the Bose–Einstein distribution, where the frequency value is given by the band-averaged frequency of each frequency band, and the temperature is the total lattice temperature, the computation of which is described in the next section.

For multidimensional structures, the methodology is similar. In 2D problems, a particular D2Q9 lattice is used and an LBKE (as in Eq. (10)) is solved for every frequency band at each time step. A numerical interpolation is then used to compute phonon distribution functions. Then, Eq. (1) is used to compute the phonon energy density at the point of interest, from which a temperature can be computed as explained in previous sections. Again, interpolation is used to compute phonon equilibrium distribution functions in the lattice sites corresponding to the spatial discretization for each frequency band. Reference [12] can be consulted for details regarding an application of LBM to 2D structures.

**Boundary Conditions: Prescribed Temperature Level.** The Dirichlet boundary condition (corresponding to a constant prescribed temperature level, which can also be a function of space and time) uses the Bose–Einstein distribution to find the phonon distribution function corresponding to the desired temperature level. In this expression, thermodynamic equilibrium is assumed at the boundary and, therefore, all the discrete phonon distribution functions along any discrete lattice direction have the same value and are given by

\[
f_i = \frac{1}{1 + \frac{\Delta t}{\tau} - 1}
\]

where \( h \) is Planck’s constant divided by \( 2\pi \), \( k_B \) the Boltzmann constant, \( T \) the lattice temperature, the subscript \( i \) the discrete lattice propagation direction of interest, the subscript \( j \) the band-averaged frequency for the \( j \)th discrete frequency band, and \( D \) the total number of discrete propagation directions in the lattice. A detailed algorithm for the dispersion LBM has been presented elsewhere [13].

**On Thermal Conductivity Computations.** When considering a gray phonon transport model [5–7], the phonon mean free path, relaxation time, heat capacity, and thermal conductivity can be related by means of the kinetic theory of gases formula given by

\[
k = \frac{1}{3} C v \Lambda \tag{11}
\]

where \( C \) is the heat capacity, \( v \) is the phonon propagation speed, and \( \Lambda \) is the phonon mean free path. Normally, bulk values for both the thermal conductivity and heat capacity are found in the literature for a range of temperatures, and the phonon propagation speed can be easily computed from the application of the Debye assumption. This makes the computation of the phonon mean free path relatively straightforward and, as a result, a Knudsen number is well defined and unique for a given system. In contrast, the dispersion LBM considers the thermal conductivity to be the sum of contributions from all phonon branches, contributions that are defined as integrals over the frequency spectrum as

\[
k = \sum_p \int C_p v_p^n \tau_p \mathrm{d}\omega \tag{12}
\]

where \( \omega \) is the phonon frequency, \( C_p \) is the frequency-dependent heat capacity, \( v_p \) is the frequency-dependent phonon propagation speed, \( \tau_p \) is the frequency-dependent phonon relaxation time, and \( p \) indicates the different phonon branches. In this case, no straightforward mathematical relation for \( \tau_p \) exists, and thus, it cannot be extracted from Eq. (12). Instead, phonon relaxation must be previously known in order to compute the value of thermal conductivity. The problem is then to find suitable phonon relaxation time expressions that can allow us to compute an accurate prediction of bulk thermal conductivity.

Traditionally, researchers have tried to predict phonon relaxation times by considering the different types of scattering events to which phonons are subject. Phonon scattering events can be divided into two categories: elastic scattering by lattice imperfections, where the incident phonon energy or frequencies are not changed, and inelastic scattering by phonon-phonon collisions. Effective phonon relaxation time values are obtained from a combination of all known phonon scattering mechanisms. This effective relaxation time can be computed by assuming that the scattering processes are independent and do not interact with each other. This assumption, although not exactly exact for inelastic scattering, can be implemented by using the Matthiessen rule.

Expressions for each type of phonon relaxation time or scattering rate can be found in several sources from the literature. For example, Callaway [14] developed his analysis based on the Debye model. This analysis does not distinguish between longitudinal and transverse polarizations and only gives good agreement with experimental data at temperatures below and around the temperature at the maximum value of thermal conductivity, but not at higher temperatures. Holland [15] extended the work of Callaway by incorporating the contributions of longitudinal and transverse phonons and using different forms for the phonon relaxation times, which result in better agreement with experimental data.
than what Callaway’s approach was able to obtain. However, in the Callaway and Holland models, there is no analytical method for predicting the values of the arbitrary constants used, and therefore closure of the model depends on fitting these parameters to previously experimental data. It has been argued [16,17] that the successful fits of experimental data in these models result from the application of proper arbitrary fitting constants and not from an accurate physics model. Moreover, this approach is only suitable for materials whose thermal properties are known. If that is the case, the experimental thermal conductivity values can be used to validate the scattering rate models (again by proper fitting of constants). Unfortunately this approach cannot be utilized for materials of unknown thermal properties since then there would be no way of properly adjusting the fitting constants.

Another shortcoming of the Debye-derived methods [14,15,18,19] results from neglecting the contribution of optical phonons. Both longitudinal and transverse optical phonons are confined to a narrow range on the frequency spectrum. This has led to the simplification presented in the Einstein model, in which both modes are collapsed into a linear dispersion curve of constant frequency. Optical modes have been modeled as to display slow propagation speeds, and at first, the Einstein model (which assigns them zero speed, that is, purely capacitive properties) seemed to be appropriate, especially in view of the extensive computational efforts required to solve a BTE that considers nonlinear dispersion for all acoustic and optical modes. However, assigning them zero propagation speed results in neglecting their contribution to the thermal conductivity, and thus, all Debye-based models focus only on relaxation time expressions for acoustic phonons. This has led to relaxation times for optical phonons receiving limited attention in the literature [20–22], and as a result there is a significant lack of anharmonic scattering expressions that could readily be used. Recently, researchers have begun to question the accuracy of this approach, and there is increasing evidence that the contribution of optical phonons to the thermal conductivity is not negligible [23–25]. Additionally, the self-heating process of silicon-on-insulator (SOI) transistors is heavily affected by optical phonon confinement within a hotspot region, and as a result, accurate relaxation time expressions for optical phonons are of critical importance in modeling the heat transport in these regions of microelectronic components [26]. Even recent research that incorporates optical phonons only does so by assuming that they are of a purely capacitive mode and assigning them zero propagation speed [8].

It is therefore clear that most approaches fail to account for the true dispersive nature of the phonon frequency spectrum. As a result, full BTE expressions for optical phonons have not been solved simultaneously to acoustic modes, and adequate expressions for the optical mode relaxation time are still lacking. This work in part addresses these issues, trying to present a novel approach to thin film heat conduction and thermal conductivity prediction by developing a model that incorporates all phonon modes in order to solve simultaneous BTE’s, in addition to considering the multiple length scale nature of the problem.

Analytical Prediction of Bulk Thermal Conductivity. As has been discussed, the only information needed to successfully simulate the thermal behavior of a crystalline structure with the LBM are adequate analytical expressions or numerical data for the dispersion relations (from which the phonon propagation speed is derived) and for the phonon relaxation times. The latter still lacking, we have resorted to compute them by implementing three-phonon interactions following the model by Han and Klemens [22]. This approach has been demonstrated to recover the bulk value of thermal conductivity for silicon [11] and seems to be adequate for our needs. However, this analysis, based on perturbation theory, relies on the assumption of low temperatures (T < 100 K) and, thus, is expected to fail at higher temperatures. Moreover, another valid alternative available is that of Sinha and Goodson [27], which presents mean free path data for bulk silicon at room temperature. In our opinion, the lack of adequate phonon relaxation time expressions is going to hinder the accuracy of our LBM method until more reliable expressions are developed. Additional details on the Han and Klemens (HK) model can be found in the literature [11,22,28]. In the model, the frequency spectrum is discretized in equal-width frequency bands, whose interaction with each other are constrained by energy and momentum conservation rules. A two-step process characterizes energy exchange between frequency bands: first, a normal process between low-wave-vector phonons and intermediate-wave-vector phonons, and then an Umklapp process between the intermediate phonons and those at the Brillouin zone. It has been argued [22,28] that important three-phonon interactions are of the types: T + L ↔ L, L + T ↔ L, and L + L ↔ L. Interactions with optical modes (T + L ↔ O, O + L ↔ O, and L + L ↔ O) are N process and cannot be included in the thermal conductivity computation. For simplicity, Narumanchi et al. [8,11] collapsed all optical modes into a single frequency band of constant frequency and zero propagation speed. Due to the intensive nature of the computational effort required to obtain frequency-dependent optical mode relaxation times, a hybrid model is proposed here: acoustic mode relaxation times are obtained from the HK [22] model, and optical mode relaxation times are those presented by Sinha and Goodson [27].

In the HK [22] model, inverse relaxation times for a specific process have the general form

\[
\frac{1}{\tau_{ij}} = \frac{a}{3\pi k_B T} \omega_i \omega_j R_{ij} \left( \frac{1}{e^{\omega_i/k_B T} - 1} - \frac{1}{e^{\omega_j/k_B T} - 1} \right)
\]

where \(\tau_{ij}\) is the relaxation time that accounts for energy exchange between the bands \(i\) and \(j\) of frequency \(\omega_i\) and \(\omega_j\), \(\omega_0\) is the intermediate phonon frequency that completes the three-phonon interaction, \(v_q\) is the phonon group velocity at \(\omega_0\), and \(v_p\) is the phase velocity of the \(i\) mode. The effective relaxation time for a discrete frequency band centered on \(\omega_i\) is found as the combination of all phonon scattering processes in a Mathiessen sense as

\[
\frac{1}{\tau_{eff,\omega_i}} = \sum_i \frac{1}{\tau_{ij}}
\]

We have compared the HK model to a hybrid model based on Han and Klemens [22] for acoustic modes, plus the addition of optical mode relaxation time data extracted from Sinha and Goodson [27]. The influence of phonon-boundary scattering in the model was tested. The bulk silicon phonon mean free path data presented in Ref. [27] is available only at room temperature, and thus the prediction of thermal conductivity with this model is possible only at room temperature. As seen in Table 1, the hybrid model seems to better predict the bulk thermal conductivity model at room temperature, displaying a percentage error of only 3.3% when compared to the experimental data of Ho et al. [29]. As a consequence, the hybrid model is adopted as the most accurate relaxation time model available for use with the dispersion LBM.

Results

In what follows, we first present time-dependent temperature profiles depicting the transition from diffusive to ballistic phonon transport in silicon thin films of decreasing thickness, obtained with the dispersion LBM. The effects of including nonlinear phonon dispersion as compared to the existing gray LBM are discussed, as well as the influence that ballistic phonon transport has

<table>
<thead>
<tr>
<th>Model</th>
<th>HK, BS</th>
<th>HK, no BS</th>
<th>Hybrid</th>
</tr>
</thead>
<tbody>
<tr>
<td>(k) (W/m K)</td>
<td>123</td>
<td>160</td>
<td>153</td>
</tr>
<tr>
<td>% error</td>
<td>16.4</td>
<td>7.8</td>
<td>3.3</td>
</tr>
</tbody>
</table>
The dimensionless temperature is $T = x/d$, where $x$ is the distance measured from the high temperature boundary, and the dimensionless temperature is $T^* = (T - T_1) / (T_2 - T_1)$.

The dispersion LBM simulation of films thicker than 1000 nm was found to be unfeasible due to the extremely high computational cost. The simulations for this work were performed in computational platforms consisting of Intel Xeon processors running at 2.20 GHz, with 8 Gb of random access memory (RAM). The system's configuration allowed us to simulate films thinner than 1000 nm. Similar to what was found by using the gray model, decreasing film thickness translates into increasing temperature slip at the boundaries, which is in agreement with results previously reported in the literature [2, 3, 5, 6, 8].

The transient dimensionless temperature profiles in a 300 nm thin film are shown in Fig. 2. Although there is some similarity with gray LBM results that fall within the diffusive regime, in this case a wave behavior can be seen at short times ($t = 11 \text{ ps}$ and $t = 30 \text{ ps}$), to be later dampened into a temperature profile that resembles diffusive transport ($t > 30 \text{ ps}$). However, the temperature slip at the boundaries is a clear indication that this case falls within the transitional regime. At steady-state conditions, the temperature profile displays a linear drop inside the film, with temperature slip conditions at each boundary.

Decreasing the film thickness by an order of magnitude results in a 30 nm thin film, whose transient dimensionless temperature profiles are shown in Fig. 3. Marked differences exist with gray LBM results. In this case, the temperature profile is composed of a combination of traveling phonon energy waves, as opposed to the single propagating wave of the gray LBM. At short times ($t = 3.47 \text{ ps}$), it can be seen that the faster acoustic phonons have propagated inside the film and are about to reach the cold boundary, while the slower but more energetic optical phonons have only begun to leave the hot boundary. Characteristic temperature slip conditions are seen in the hot boundary. As time advances, all acoustic phonon waves have already reached the cold boundary, and only the slow optical phonon waves still propagate ($t = 37.6 \text{ ps}$). Finally, steady-state conditions are achieved, the temperature profile displays slip conditions at both boundaries and a linear drop inside the thin film.

Figure 4 shows the transient dimensionless temperature profiles in a 3 nm thin film, which is considered to be the lower limit at which an LBM can be applied; the film thickness is on the order...
of phonon wavelengths and, therefore, a molecular approach is needed to perform thermal analysis below this thickness. Marked differences exist with gray LBM results. In this case, the temperature profile is composed of a combination of traveling phonon energy waves, as opposed to the single propagating wave of the gray LBM. At short times ($t=0.175$ ps), it is clearly seen that faster acoustic phonons have propagated inside the film and are about to hit the cold boundary, while slower but energetic optical phonons have only begun to leave the hot boundary. Characteristic temperature slip conditions are seen in the hot boundary. As time advances, all acoustic phonon waves have already reached the cold boundary, and only slow optical phonon waves propagate ($t=3.1$ ps). Finally, steady-state conditions are achieved and the temperature profile displays slip conditions at the boundaries and a linear drop inside the thin film.

The temperature slip condition can be explained by observing that constant temperature levels at the boundaries have the net effect of enforcing an emission of phonons with an energy density corresponding to the imposed boundary temperature. As the frequency-dependent band Knudsen number for a given frequency band approaches a value that situates the frequency band within the subcontinuum regime, the phonons traveling toward the boundary have a significantly different energy density than that of the phonons emitted from the boundary, therefore resulting in an abrupt change in energy density, which displays itself as the temperature slip at the boundaries. The magnitude of the temperature slip at the boundary is proportional to the Knudsen number, being zero in the limit of a vanishing Knudsen number, as occurs for a purely diffusive regime, characteristic of Fourier conduction. Thus, in the context of the dispersion model, each frequency band displays a temperature slip whose magnitude is given by the band Knudsen number and thus represents a band thermal resistance. The total thermal resistance of the superimposed temperature slip conditions is to be given by the final temperature profile and the magnitude of the boundary temperature slip.

One interesting characteristic of the dispersion LBM model, a fundamental difference with the gray LBM, is the coexistence of different transport regimes for a given film thickness. Here, we define a frequency-dependent band Knudsen number as $\text{Kn}(\omega) = \Lambda(\omega)/d$, where $\Lambda(\omega)$ is the frequency-dependent phonon mean free path and $d$ the film thickness. The diffusive regime is defined for a very small or vanishing Knudsen number, which can be arbitrarily expressed as $\text{Kn}(\omega) < 0.01$, with the other limit being the purely ballistic regime, defined as $\text{Kn}(\omega) > 100$. To illustrate this point, Fig. 5 depicts the band Knudsen number for all phonon branches in a film of 1000 nm thickness, as a function of phonon frequency. The figure normalizes the phonon mean free path data for silicon presented in Fig. 13 from Ref. [27] by dividing it with the film thickness of 1000 nm.

It is observed that only the lowest-frequency LA bands, which happen to propagate at the fastest speeds of the phonon system, are located at a Knudsen number range that characterize them as being within the purely ballistic regime. Higher-frequency LA bands are mostly located within the transitional regime, except for the bands the with highest frequency, which are located at Knudsen numbers characteristic of the diffusive regime. TA and LO branches have both a band Knudsen number range within the transitional and diffusive regimes, while most TO bands are well within the diffusive regime. The implications of this behavior are twofold: First, at a film thickness that in the gray LBM could be located close to the diffusive regime, the dispersion model presents results that are shifted toward the transitional regime. Second, the transition to ballistic regime is likely to be a process that occurs at a wider range of film thicknesses due to the order-of-magnitude differences in band Knudsen number range for all branches. This basically implies that energy transport in a film of a given arbitrary thickness is likely to display characteristics of at least two, if not all three, of the transport regimes.

Validation of the Dispersion LBM. The task of performing dispersion LBM simulations within the diffusive regime is indeed formidable. The multiple LBKEs that need to be simultaneously solved, each having its own lattice spacing, make the task of reaching the diffusive regime a most difficult enterprise. Considering the required computational effort, a direct validation of the dispersion LBM in the diffusive regime, by comparing with Fourier diffusion solutions, is not feasible under the current structure of the dispersion LBM code. The first resulting recommendation is to avoid the use of LBM, in any of its forms (gray and dispersion), for the simulation of diffusive regime problems. For this, traditional techniques based on discretization of the Fourier heat conduction equation are more efficient, which limits the use of LBM-based techniques to the transitional and ballistic regimes. The second recommendation is to embark in a revision and modification of the current code in order to make it more efficient and able to simulate a broader range of length and time scales. Incorporating parallel computing capabilities to the LBM code is part of the author’s ongoing work.

Thickness-Dependent Thermal Conductivity. As we have seen, the analytical model used for selecting the appropriate expressions of phonon mean free path for the dispersion LBM was able to recover the thermal conductivity value for bulk silicon...
with an acceptable accuracy. To further analyze the dispersion LBM capabilities, this section presents results for thermal conductivity as a function of film thickness of the one-dimensional model based on the steady-state temperature distribution displayed in the previous section. To compute the effective size-dependent thermal conductivity, it is necessary to first know the heat flux being transported across the film and the magnitude of the temperature slip.

The heat flux can be computed by using a general expression of heat flux, applying it to each discrete frequency band for all phonon modes and then adding their contributions, as given by

\[ q_{\text{LBM}} = \sum_p \int_{\Delta \omega_p} v_i \tau_{\text{LBM}}(\omega) d\omega \]  

(17)

The bulk value of thermal conductivity is known from Eq. (14) and Table 1. This value is used in Eq. (18) to find the frequency-dependent effective thermal conductivity, and the total effective thermal conductivity is computed as the sum of all frequency-dependent contributions of all phonon modes,

\[ k_{\text{effective}}(\omega) = \frac{k_{\text{bulk}}}{1 + 2CKn(\omega)} \]  

(18)

where \( C \) corresponds to a geometric parameter that takes into account the magnitude of the boundary temperature slip [30].

Figure 6 depicts a comparison between out-of-plane effective thermal conductivity predictions by the gray and dispersion LBMs. As can be seen, the gray LBM predicts an effective thermal conductivity value that remains close to the bulk value of 148 W/(m K) down to a film thickness of 1000 nm. Further decreases in the film thickness cause a slight decrease of the effective thermal conductivity down to a film thickness of approximately 400 nm. For films thinner than 400 nm, the decrease on thermal conductivity is more pronounced and the gray LBM eventually predicts a zero thermal conductivity value for a film of vanishing thickness. This behavior is consistent with the gray LBM formulation, in which the transition to ballistic transport is a function of a single parameter, the Knudsen number. Subcontinuum effects start to influence the energy transport process at Knudsen numbers of about Kn = 0.1, corresponding to a film thickness of 410 nm. The transition to ballistic transport occurs between Kn = 0.1 (for film thickness of d = 410 nm) and Kn = 10 (for film thickness of d = 4.1 nm), a phenomenon that is manifested by the reduction of effective thermal conductivity value.

Following what was expressed in previous sections, the analytical dispersion model gives a bulk thermal conductivity value of 153 W/m, which compares well with the value predicted by the gray LBM, 145 W/m K, and is in good agreement with the experimental value of 148 W/m K. As we have mentioned, reaching the diffusive regime with the dispersion LBM would involve the simulation of films with thickness in the order of millimeters, which does not compare well with the actual capabilities of the LBM code, as the limit for feasible simulations was found to be about 1000 nm. Thus, we are prevented from reaching a purely diffusive regime and have instead computed effective thermal conductivity values for film thickness below 1000 nm.

As seen in Fig. 6, the thickness-dependent effective thermal conductivity predicted by the dispersion LBM is consistently lower than that predicted by the gray LBM. The dispersion model predicts an earlier shift from the diffusive transport regime to the transitional regime, a situation that arises from phonon frequency bands clearly residing in the transitional transport region (Fig. 5), this, even for a film thickness that the gray model had characterized as being very close to the diffusive regime. Further reducing the film thickness results in more phonon frequency bands being located within the transitional regime, and as a result, the general trend is for the dispersion LBM to predict values of effective thermal conductivity lower than the gray LBM. As for the physical mechanism that results in the effective thermal conductivity being lower than the bulk value, this is thought to be due to strong phonon-boundary scattering, where phonons traveling to and from the prescribed temperature boundaries are forced to suddenly change their energy density, which induces the boundary temperature slip conditions observed in Figs. 1–4. Although it is somewhat difficult to validate the results for our 1D model, in the limit of large length scales the dispersion LBM is able to recover the bulk value of thermal conductivity, and in the size effect regime they compare well to those presented in Refs. [16,17,22–25,28].

**Conclusions**

The dispersion LBM is used to study the transition to ballistic transport in silicon films of varying thickness. It is found that for large length scales, it is found that simulating the transition to diffusive transport is unfeasible due to the large domain sizes required, which are in the order of millimeters. This is again a result of most frequency bands being located within the transitional regime even for that reduced thickness. On the other extreme of large length scales, it is found that simulating the transition to diffusive transport is unfeasible due to the large domain sizes required, which are in the order of millimeters. This is again a result of most frequency bands being located within the transitional regime for film thickness deemed within the diffusive regime by the gray LBM. As a consequence, the thickness-dependent effective thermal conductivity values predicted by the dispersion LBM are consistently lower than those predicted by the gray LBM for the same film thickness. The dispersion LBM, which includes the effects of nonlinear dispersion relations for all phonon branches, is considered to be more accurate than the gray LBM due to the improved phonon physics inherently captured by the model, which allows the simulation of multiple discrete phonon frequency bands and the explicit treatment of optical phonons without simplifying assumptions. This is a considerable improvement from the Debye-based gray LBM, which only considers a single phonon mode with a constant propagation speed and is therefore unable to capture the behavior of phonon modes characterized by propagation speeds different from the one defined by the Debye model.

**Acknowledgment**

The authors gratefully acknowledge support from the National Science Foundation Grant No. CTS-0103082, the ICES Pennsylvania Infrastructure Technology Alliance (PITA) Program sponsored by the Commonwealth of Pennsylvania’s Department of Community and Economic Development, the Pontificia Universidad Católica de Chile, and the Chilean Fondo Nacional de Ciencia y Tecnología (FONDECYT), through Grant Nos. 1050087 and 11030620.
References