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Comparative assessment of deterministic approaches to modeling quasi-ballistic phonon heat conduction in multi-dimensional geometry

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ABSTRACT

When the mean free path of the dominant energy carriers in semiconductor materials, namely phonons, is comparable to or larger than the characteristic length scale, scattering of phonons is rare, and the equilibrium Bose-Einstein distribution is not restored locally. Four different models for modeling non-equilibrium (or quasi-ballistic) heat transport in multi-dimensional geometry are critically assessed in this study. These include (1) the hyperbolic heat equation (HHCE), (2) the first-order method of spherical harmonics or P_1 approximation (P1), (3) the frequency-dependent phonon Boltzmann Transport Equation (BTE), and (4) a hybrid approach in which the BTE is hybridized with the P_1 approximation (Hybrid). In addition, the Fourier law (Fourier) is also considered to assess its regime of validity. A two-dimensional sub-micron heat conduction problem is solved using all of the aforementioned models, and their accuracy and efficiency are assessed. The full BTE solution with high spatial and angular resolution is considered the benchmark solution for comparison. Both steady and unsteady computations are conducted. It is found that at steady state, the accuracy of the models go hand in hand with the degree of diffuse approximation incorporated into the model. At low temperature, where the degree of non-equilibrium (ballistic nature) is dominant, the Fourier model completely fails. For transient computations, at short times, all models other than the BTE exhibit significant error. Also, the HHCE is found to be significantly superior to the Fourier model at short times.

1. Introduction

Typical feature sizes or characteristic length scales in modern-day electronic and optoelectronic devices range between 10 and 100 nm. Phonons, which are the dominant energy carriers in semiconductor materials, have spectral mean free paths that overlap with this range. For example, the mean free path of phonons in silicon at room temperature is in the range 10–10^4 nm, with the estimated mean around 300 nm [1]. Consequently, heat conduction in such solid-state devices cannot be described adequately using continuum transport equations, most notably the Fourier law of heat conduction.

When the phonon mean free path is significantly larger than the characteristic size of the system under consideration, phonons rarely scatter, and their transport is so-called *ballistic*. In the ballistic regime, the Knudsen number, which is the ratio of the mean free path of the phonon to the characteristic length scale, is large, *i.e.*, $Kn \gg 1$. On the other hand, when the phonon mean free path is small in comparison to the characteristic size of the system, they undergo numerous scattering events, resulting in so-called *diffusive* transport. In this case, $Kn \ll 1$. In the ballistic regime, the energy flux in a given direction (or intensity) may be very large along directions that directly connect hot and cold entities, while it may be small in other directions. Consequently, ballistic transport is strongly direction dependent. Since scattering re-distributes energy directionally, abundant scattering, as is prevalent in the diffusive regime, makes the intensity more or less isotropic or direction independent. Therefore, one may conclude that when scattering is infrequent, as in the case of ballistic transport, the directional nature of phonon transport needs to be considered carefully. Conversely, when scattering is dominant, the directional nature of phonon transport is weak. The Fourier law of heat conduction essentially assumes that phonons have vanishingly small Knudsen number, and consequently, a perfectly isotropic intensity field locally. This phenomenological law is purely diffusive and is based on the linear gradient diffusion hypothesis [2]. It does not account for the wave nature of phonon transport and is incapable of predicting heat conduction in the mixed ballistic-diffusive (or *quasi-ballistic*) regime of transport, which is the primary focus of this discussion.

Another major shortcoming of the Fourier law is that it disregards

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the finite propagation speed of the phonons. When the characteristic time-scale (time taken by a phonon to traverse the characteristic length of the system under consideration) is comparable to or smaller than the phonon relaxation time-scale, the speed of propagation of the phonon becomes relevant. In an effort to accommodate finite carrier (phonons in the case of semiconductors) propagation speeds into heat transport models, the Cattaneo equation [3–5] was proposed, which, in combination with the first law of thermodynamics (energy conservation) results in the so-called hyperbolic heat conduction equation. The hyperbolic heat conduction equation has been used extensively in heat transfer analysis, especially in scenarios where pulsed heating or cooling is prevalent. Another variation of this equation is the so-called dual phase lag model [5].

Although the hyperbolic heat conduction equation accommodates finite carrier speed and has the potential to treat quasi-ballistic thermal transport, it is still not adequate for the treatment of phonon-mediated thermal transport in semiconductors. This is because, as insinuated earlier, phonons in semiconductors have a large range of frequencies, and consequently, different group velocities and scattering rates. Hence, a single relaxation time-scale, as appearing in the hyperbolic heat conduction equation, is not adequate to capture the combined effect of all phonons. Some phonons may be ballistic, while others may be diffusive. Thus, although the hyperbolic heat conduction has been in existence for more than half a century, it has found limited use for predicting phonon mediated thermal transport in semiconductor applications.

The Boltzmann Transport Equation (BTE) for phonons [3] adequately captures the mixed ballistic-diffusive nature of phonon transport in semiconductors. It describes the spatio-temporal evolution of the number density of an ensemble of phonons (or the energy carried by the ensemble) of different frequencies as these phonons engage in free flight and scattering. Incidentally, both the Fourier law and the Cattaneo equation can be derived from the BTE under a number simplifying assumptions, some of which have already been mentioned earlier. The Fourier law represents the zeroth moment of the BTE while the Cattaneo equation represents the first moment. The phonon BTE is an integro-differential equation in 7 independent variables: time, 3 spatial coordinates, and 3 wave-vector coordinates. For an isotropic wave-vector space, the 3 wave-vector coordinates may be reduced to 2 directional (or angular) coordinates, and frequency. Furthermore, under the single-time relaxation approximation, the scattering term of the BTE can be significantly reduced (linearized) resulting in a 7-dimensional partial differential equation. Even the linearized BTE, however, is challenging to solve because of its high dimensionality. A number of methods have been used to date to numerically solve the phonon BTE. These include the Monte Carlo method, the lattice Boltzmann method, and deterministic discretization-based methods. The Monte Carlo method is suitable for the inclusion of complex physics such as dispersion, polarization, and various scattering mechanisms [6–10]. However, it is expensive for practical engineering applications, especially when high spatial resolution is sought. Recently, variance reduction techniques have been adopted for phonon transport, thereby enabling Monte Carlo simulations of phonon transport in realistic three-dimensional structures [11]. To date, the lattice Boltzmann method has found only limited use [12,13].

Deterministic solution of the phonon BTE is based on discretization in all 7 dimensions [14–17]. In such methods, spatial discretization is performed using either the finite difference, the finite element or the finite volume method [18], while angular discretization is performed using the discrete ordinates method and its variant, namely the control angle discrete ordinates method [19,20]. The finite volume method is generally preferred over the other two methods for spatial discretization since it guarantees flux conservation, while the control angle discrete ordinates method (CADOM) is preferred over the standard discrete ordinates method since it mitigates ray effects [19–21]. Until recently, the solution to the three-dimensional (3D) frequency-dependent (or non-gray) phonon BTE has been prohibitive due to the extreme memory and computational time requirements. Earlier studies [22] and some recent studies [23] have reported solution to the two-dimensional (2D) non-gray BTE with the goal to understand hot spot generation and dissipation in device-like structures. Very recently, Mazumder and co-workers [24,25] have demonstrated solution to the full non-gray BTE in 3D heterostructures discretized using an unstructured mesh. The 2D non-gray BTE has also been used to mimic time-domain thermo-reflectance experiments by the same group [26], wherein extremely short time-scale phenomena need to be resolved. The most notable recent work on the solution of the 3D non-gray BTE is the one reported by Ali et al. [24], who demonstrated solution to the phonon BTE in a 3D device-like structure discretized using 604,054 tetrahedral control volumes, 400 angles, and 40 spectral intervals (or bands), resulting in 9.7 billion unknowns. These computations were performed using 400 processors in parallel, and required 156 GB of RAM and 1.1 h per time step. These extreme computational requirements are indicative of the fact that although it is now possible to solve the 3D non-gray BTE in systems of practical interest, the computations are still extremely time-consuming.

While it is possible to reduce computational times further by capitalizing upon ongoing advances in high performance computing, what is incumbent is the development of methods for solving the BTE that capitalize upon the physics of phonon transport to improve efficiency of solution. To this end, several approaches have been recently explored. The fundamental premise that in the ballistic regime, the phonon intensity is strongly directional, while in the diffusive regime it is more or less isotropic, has been used to develop hybrid solution strategies for the BTE. One of the earliest hybrid solution strategies to the BTE was proposed by Chen and co-workers [27–29]. In their approach, the phonon intensity was assumed to be a superposition of a ballistic intensity and a diffusive intensity. The diffusive intensity, by virtue of being isotropic, was determined by invoking the method of spherical harmonics. The resulting model is the so-called ballistic-diffusive equations (BDE) of phonon transport. In the BDE formulation [27–29] proposed by Chen and co-workers, the diffusive component was determined using a standard elliptic partial differential equation solution procedure, while the ballistic component was determined using the surface-to-surface exchange formulation and geometric viewfactors [29], which makes the method somewhat restrictive for complex geometries. Mittal and Mazumder [30,31] developed an alternative formulation, in which the ballistic component of the phonon intensity is determined instead using the CADOM, making the solution algorithm amenable to large-scale computations in complex geometries. The method has been successfully demonstrated for the solution of the transient BTE in complex 3D nanostructures [31]. Both of the aforementioned hybrid methods were demonstrated for the gray (frequency independent) BTE only, and important physics pertaining to phonons, namely dispersion and polarization effects, were not considered. In an effort to include such relevant physics while improving computational efficiency, ballistic-diffusive hybridization of the frequency-dependent (non-gray) phonon BTE has also been pursued by some researchers. Loy et al. [23] proposed a strategy in which the Fourier law is directly used for frequencies for which the spectral Knudsen number is small, and the full BTE for frequencies for which the spectral Knudsen number is large. The model has been referred to as the hybrid Fourier-BTE model [20]. Recently, Allu and Mazumder [32] proposed a similar hybridization strategy, with the exception that in their formulation, in the diffusive regime, the Fourier law is not used. Rather the first-order method of spherical harmonics (P_1 approximation) is invoked to reduce the BTE. In the P_1 approximation, the phonon intensity is not assumed to be perfectly isotropic (independent of direction), but rather, linearly varying with direction. This extension embodies weak directional variations of the diffuse component of the phonon intensity, and is more appropriate since perfect isotropy of the intensity is only an idealization. Another hybrid model that has been proposed is the so-called