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A multiscale thermal modeling approach for ballistic and diffusive heat transport in two dimensional domains

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ABSTRACT

The modeling of heat transport for small length scales requires accounting for the physics of heat carrier transport such as the propagation, scattering, and relaxation of phonons. However, the models used to describe such phenomena are often too computationally expensive to model large domains where relevant system boundaries are far removed from the region where ballistic-diffusive phonon transport is dominant. To address the response of such systems to its far field thermal boundary conditions, a multiscale thermal model is needed to efficiently account for transport phenomena in each domain. In this work, a multiscale thermal modeling approach is presented where the transport of phonons is treated with a Finite Volume Discrete Ordinates Model (FVDOM) solution to the phonon Boltzmann Transport Equation (BTE) which is embedded in a region treated by diffusive thermal transport. The approach shows that it is possible to create a coupled multiscale model where the boundary conditions of the FVDOM model are derived from the diffusive transport model. The limitations of the method and the key parameters for accurate modeling are investigated and discussed. The final model is used to explore the impact of the size of heat generation regions with respect to the overall domain size on the peak temperature. The results show that by using such a model it is possible to capture the ballistic-diffusive transport in pertinent areas of a domain that is mostly dominated by diffusive transport.

1. Introduction

Thermal transport at small length scales has become of great technological importance in understanding the thermal behavior of systems such as microelectronics, MEMS, and nanoscale systems. In the area of microelectronics, the process of joule heating and the formation of hotspots often occur on length scales that are on the order of or smaller than the mean free path of the dominant heat carriers (phonons). The transport of heat in such domains has been addressed before by researchers studying silicon and III-nitride transistor devices and has been shown to result in temperatures higher than those predicted by diffusive heat transfer models [1–4]. In field effect transistor devices such as metal oxide semiconductor field effect transistors (MOSFETs) and heterostructure field effect transistors (HFETs), high electric fields near the drain side of the gate accelerates electrons through the device channel. The high energy electrons cause phonon emission through Fröhlich interactions and induce hotspots formation on the drain side edge of the gate [4–6]. In such cases, the intense heat generation region can have dimensions on the order of tens of nanometers [1,7]. For materials like Si where more than 50% of the heat is carried by phonons with mean free paths smaller than 10–20 nm at room temperature [8,9], such heat generation zones raise the question the validity of diffusive transport models to describe these peak temperatures. Previous studies performed on such devices showed that ballistic phonon transport plays an important role in heat transport and modeling this phenomena result in temperatures higher than those predicted by conventional diffusive heat transfer models [1–4].

The ballistic phonon transport effects are responsible for temperatures higher than temperatures predicted by Fourier's diffusion theory. These effects can be accounted for in device modeling by solving the phonon Boltzmann transport equation (BTE) [10]. The phonon BTE describes the rate of change of the statistical distribution function for phonons and is given as [11]:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \left(\frac{\partial f}{\partial t}\right)_{scatt} \quad (1)$$

where f is the phonon distribution function, $\vec{v}$ is the phonon group velocity based on the dispersion relationship. The scattering term on the right hand side represents the change in particle distribution

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function due to the energy carrying particle collisions with other phonons, isotopes, electrons, and crystal defects. This equation has been used previously for the thermal modeling of semiconductors [2,4,12,13]. The distribution function *f*, is a function of position, direction, frequency and polarization of a phonon. Therefore, the solution of Eq. (1) is not straightforward and is often computationally expensive.

The solution of the phonon BTE can be approximated by using a Monte Carlo simulation approach [14]. However, due to the large number of collision interactions that must be computed, Monte Carlo simulations are difficult to perform for domains with length scales greater than 1 μm [15]. Numerical solutions of the phonon BTE are feasible to implement and permit the analysis of complex domains with varying boundary conditions and heat generation if the relaxation time approximation is used [10]. Numerical techniques such as finite difference lattice Boltzmann method (LBM) and the finite volume discrete ordinates method (FVDOM) have been used to solve BTE given in Eq. (1) for semiconductor devices [1,2,16,17]. In LBM, phonons are allowed to propagate only along the grid lattice directions, thus LBM is not successful in eliminating the "ray effects" that arise from using a limited number of phonon propagation directions [15]. Unlike LBM, the spatial and angular discretizations of the domain are independent of each other in DOM. Therefore, DOM is a better method to obtain accurate results when ballistic transport effects are present since "ray effects" can be removed almost entirely [15].

As a result, DOM is chosen in this study for the angular discretization and control volume approach is used for the spatial discretization. This technique is called "Finite Volume Discrete Ordinates Model (FVDOM)" and it can be used to investigate the ballistic-diffusive effects of phonon transport. However, modeling the entire geometry is computationally expensive since FVDOM should be solved for all nodes and directions of phonon propagation. As an example, the number of degrees of freedom of a 2D problem increases 1,000,000 times when the size of the domain to be modeled is increased to millimeter range from micrometer range using uniform mesh. Considering that the number of equations to be solved for each node is equal to the number of phonon propagation directions (which can vary from 12 to 40 (S4–S8 Quadratures) in 2D) the computational cost of the problem increases significantly.

Due to these computational challenges, many previous simulations have been limited to domains where only ballistic-diffusive phonon transport effects are present. However, this may lead to the exclusion of the effects of the far field system boundaries that can impact the system level and local level responses. In order to include far field system boundary effects with reasonable computational cost one can use non-uniform mesh. However, to do this the model should be significantly changed. Moreover, it will be redundant to solve BTE for elements that are big enough and far away from the ballistic effects since they can be modeled with diffusive models.

To overcome these computational issues, a multiscale model is necessary. Multiscale methods are generally built by partitioning the domain into two regions. In regions that are far from the heat generation, ballistic-diffusive phonon transport is not important due to sufficient phonon scattering events. For these regions, diffusive transport models are used to describe the thermal response that can be easily solved using a number of numerical approaches including finite elements and finite difference methods. However, such models do not capture the increased temperature in the heat generation region where phonon transport physics becomes important. Thus ballistic-diffusive phonon transport equations are solved in heat generation regions.

Several groups have implemented various multiscale solutions solving ballistic-diffusive phonon transport in a small domain of interest, while addressing the remaining portions of the system using a diffusive transport model [18,19]. However, a systematic study including the limitations of such multiscale models in evaluating the domains with localized hotspots has not been investigated in detail. In this paper a coupled phonon BTE and a Fourier diffusion equation solver will be introduced and a systematic study of its limitations when applied to domains with localized heat generation will be investigated.

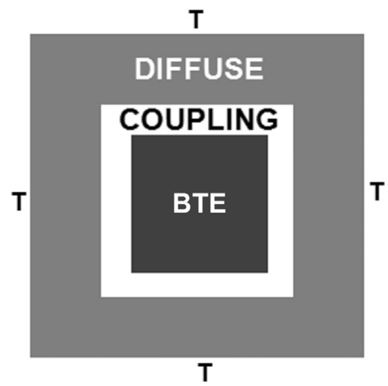

Fig. 1. Domains of multiscale Fourier-phonon BTE solver. The BTE region is where phonon BTE is solved, the diffuse region is where Fourier's heat diffusion equation is used, and the coupling region represents the region where these two regions are coupled to each other.

2. Multiscale thermal model

Previous studies have shown that ballistic-diffusive effects present in the vicinity of a heat generation region smaller than the phonon mean free path will cause higher peak temperatures to occur within the hotspot region, but far removed from this region, the temperature response will relax to one described by Fourier diffusion [6]. Since heat transport becomes diffuse after a certain distance, it is redundant and computationally expensive to model such far field areas using phonon BTE solutions. As a result, a multiscale model that involves partitioning of the domain into two sub domains as illustrated in Fig. 1 is proposed. The inner domain includes the heat generation region where the ballistic-diffusive effects are dominant and is thus referred to as the BTE domain. An outer domain that contains the rest of the geometry where ballistic effects are negligible is called the Fourier domain. The two domains are coupled together at coupling nodes where the temperature and energy fluxes must be equal. The discretization of the relevant thermal transport equations required for the numerical simulations and the coupling techniques will be explained in the next section.

2.1. Solution in the BTE domain

The Discrete Ordinates Method (DOM) [20–22] is the technique used for the angular discretization and solution of the phonon BTE in the BTE domain. Discretization is performed using the simplified steady state energy form of Eq. (1) [23]:

$$\nabla\cdot\vec{v}_g e = \frac{e^0 - e}{\tau} + q''' \tag{2}$$

where e is the energy density per unit solid angle, $\vec{v}_g$ is the group velocity, τ is the relaxation time, e^0 is the equilibrium energy density, and q''' is the phonon energy source term. Energy form of