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An anisotropic full Brillouin zone model for the three dimensional phonon Boltzmann transport equation

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Highlights

- Computational method for 3D anisotropic phonon and thermal transport.
- Full Brillouin Zone modeling with Born von-Karman boundary conditions.
- Differences in temperatures between anisotropic and isotropic behavior 10%-28%.
- Study of joule heating effects in fin field effect transistor.

Abstract

A model and associated numerical method are presented for simulation of heat transport at the microscale via the solution of the three dimensional phonon Boltzmann Transport Equation (BTE). In small domains, the full Brillouin Zone has a finite number of vibrational modes, as determined by Born von-Karman boundary conditions. As a result of this discreteness, the present method allows for general crystal anisotropy and finite dimensional effects that naturally permit anisotropic thermal transport and energy flow. The method is shown and verified using analytical solutions for isotropic flows. Then numerical experiments are performed to calculate temperature and energy in a fin field effect transistor made of a cubic crystalline material. The anisotropic thermal conductivity and the consequences on thermal fields are calculated. The differences between an isotropic solution and the anisotropic model are shown to be significant with differences in the temperatures approximately 10%. At larger scales, where scattering effects dominate, differences in the solutions become smaller and macroscopic isotropy is recovered due to the cubic symmetry of the material.

Keywords: Phonon; Boltzmann; Heat transport; Anisotropic; Three dimensional

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1. Introduction

Continuum descriptions of heat transport, such as Fourier's Law, break down at length scales on the order of the phonon mean free path (MFP). Whereas the MFP in monocrystalline silicon at ambient conditions is 300 nm [1], transistor devices made of silicon now have feature sizes of less than 100 nm [2]. At such length scales, thermal transport is not purely diffusive. Furthermore, the small finite-sized device structures limit the number of carriers—the set of carriers that can transport energy is discrete [3]. Thus anisotropy of transport can occur from the macroscopic anisotropy of the crystal structure in, for instance, hexagonal crystals [4], from the discreteness of the lattice and the reduction in the number of carriers due to finite dimensional sizes [3], and also anisotropy of dispersion within the Brillouin zone. Crystal anisotropy produces radially nonsymmetric dispersion surfaces and group velocities which then directionally-biases thermal carriers. The truncation of the lattice into a domain with orthorhombic shape results in an unequal number of carriers in those directions. Computational approaches applied to such problems must therefore be capable of modeling discrete and anisotropic carriers in both the ballistic and diffusive transport regimes. The phonon Boltzmann Transport Equation (BTE) is well-suited to this task. It is capable of accurately determining phonon transport in devices with dimensions on the order of a phonon MFP [5].

The need for modeling phonon and energy transport at the nanoscale also continues to increase as a result of both emergent vertical device geometries [6] and reductions in device dimensions [7]. Earlier computational studies were focused on two-dimensional structures primarily directed towards horizontal devices [8–12]. Recent studies have also found that anisotropic effects play an important role in heat flow in silicon nanomembranes and layered graphite thin films [13,14]. Current computational approaches appear to employ assumptions that do not make it obvious how they should be extended to consider anisotropic mechanisms. Prevailing methods employ an isotropic assumption where phonon behavior along a single high symmetry line of the Brillouin zone is taken to model the phonon properties in all directions [15–17]. Thus isotropy has a radially symmetric model of the Brillouin zone which necessarily produces a diagonal conductivity tensor with equal terms. It cannot consider situations encountered in general anisotropic thermal flows where the conductivity tensor has non-zero off-diagonal terms or non-equal terms along the diagonal, or both.

Early computational approaches for solving the phonon BTE were directed towards study of solids composed of group-IV chemical elements whose bonds are generally tetrahedrally-coordinated. Owing to this symmetry, the macroscopic thermal conductivity is isotropic. Thus the first computational methods assumed that phonons could take on the same frequencies in any direction, usually based on the frequencies in a high symmetry direction as described earlier, and therefore exhibit isotropy in their flows. For instance, Mazumder and Majumdar developed a Monte Carlo (MC) solution method for the two dimensional phonon BTE, which accounted for dispersion and multiple acoustic branches along a single direction in the Brillouin zone [10]. The method was used to determine thermal conductivity values in thin silicon films which were found to agree well with experimental values. Narumanchi et al. developed a control volume method for the solution of the two dimensional phonon BTE [8] and similarly found good agreement in conductivity values with experimental results for a range of film widths and dopant levels in silicon. Ali and Mazumder developed a technique for the solution of the three dimensional phonon BTE in a heterogeneous material which accounted for material interfaces [16]. Their model incorporated phonon scattering at material interfaces as well as variation in the dispersion relations in the two materials.

In transport of energy in finite dimensional structures, the discreteness and truncation of the lattice lead to discreteness of carriers and, therefore, anisotropic thermal flows. A general cubic crystal therefore should exhibit anisotropy in small device structures, namely in the ballistic regime, but isotropy at large scales in the diffusive regime [18]. Ni and Murthy accounted for the anisotropy of phonon properties in a continuous representation of the Brillouin zone BTE [12]. While anisotropy could be modeled through this approach, a continuous Brillouin zone largely confines that consideration to macroscopic anisotropy. The anisotropic features allowed them to also model anisotropic phonon scattering through directionally-dependent relaxation times.

In this paper, a method is presented for three dimensional solutions to the phonon BTE with explicit consideration for the physically allowed phonon modes in finite dimensional structures. Also, despite the widespread availability of BTE solvers and descriptions of solution methods, it is remarkable that few if any computer methods have been described. Our goal is to investigate the role of crystal anisotropy on thermal transport and draw conclusions about their effects. This paper details the computer methods while explicitly considering the physically allowed phonon modes using Born Von-Karman boundary conditions. The method is described in Section 3 and then verified in Section 4.1 using an emulated isotropic condition that is compared with an analytical radiative transport solution. Finally