140e Anisotropic Thermal Transport Estimation in Semiconductor Thin Films Via Lattice Boltzmann Method

Sartaj S. Ghai, Woo Tae Kim, Cristina H. Amon, and Myung S. Jhon

To achieve faster and smaller devices, regular advancements in microfabrication techniques have been achieved which has resulted in the device characteristic length to approach nanometer scale. At this nanoscale dimension, materials start to act characteristically different in comparison to the bulk system. This considerable change in the behavior results from the onset of sub-continuum regime where the long established continuum based models break down and more rigorous physics is required to capture the sub-continuum behavior of the system.

An important case where the sub-continuum effects are playing a critical role is the thermal transport in the nanoscale confined semiconductor films in the state-of-the-art electronic devices. In these devices, an increased emphasis has been laid on achieving smaller and faster systems, which has forced their characteristic length to nanometer scale. At these scales the sub-continuum effects of ballistic thermal transport, temperature slip at the boundaries, and anisotropic thermal conductivity become very prominent and energy management plays a crucial role in the operation and reliability of the system.

Continuum based Fourier equation have been proved inadequate to describe these phenomena and a rigorous physics based model, e.g., Boltzmann transport equation (BTE), which can accurately capture these effects, is required. The BTE is based on phase-space formulation and thus is computationally quite intensive. This has lead to the development of an alternative model, stemmed from BTE, lattice Boltzmann method (LBM), to successfully capture the transient thermal profile at a reduced computational cost. The virtues of being inherently transient, easy to hybridize with other physical models and length scales, and inherently parallel in nature made LBM as our natural choice.

In sub-continuum domain the boundary conditions become very significant and they govern the effective mean free path of the carriers and thus control the transport properties of the solid. At the boundary, energy carriers are scattered both specularly and diffusively. Therefore, we incorporated a surface scattering factor, which is the fraction of carriers undergoing diffusive scattering at the boundary, and studied the thermal conductivity and temperature slip at the solid boundaries.

Using LBM, we studied silicon thin films of varying thicknesses ranging from few tens of nanometers to a few microns and observed that the thermal conductivity and temperature slip at the boundaries depends strongly on the surface scattering factor and the geometric dimensions in addition to the temperature of the film. Strong anisotropy in thermal conductivity and big temperature jumps at the boundaries has been observed for the thin films of silicon, which exhibits isotropic thermal behavior in the bulk. We constructed equations which can successfully model the anisotropic conductivity and temperature slip as a function of surface scattering factor and the thickness of the film. These expressions predict the numerical solution of LBM very closely and can act as correction terms for the existing numerical solvers based on Fourier equation.