VFF-Monte Carlo Framework for Phonon Transport in Nanostructures

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ABSTRACT

Accurate modeling of non-equilibrium heat transport in nanostructures demands an appropriate description of phonon dispersion relation and proper treatment of various anharmonic effects. In this work, we develop and employ a coupled VFF molecular mechanics-Monte Carlo (VFF-MC) platform to solve the phonon Boltzmann Transport Equation (BTE) for modeling thermal conductivity in nanostructures having specified geometry.

SIMULATION MODEL

Modeling phonon transport via the BTE is adopted when the scattering rates of phonons that determine the thermal conductivity vary significantly within a distance comparable to their respective mean free paths. In this regard, the ability of the particle based Monte Carlo (MC) method to emulate the phonon behavior and introduce randomness as close to reality has further favored the use of MC based simulation in the recent years. The Ensemble Monte Carlo (EMC) scheme adopted in this work is similar to the one described in Refs. [1][2]; yet the current work stands out owing to its use of atomistically obtained dispersion relations, which serve as input for the aforementioned MC simulation. Fig. 1 illustrates the MC schema adopted in this work. The dispersion relation (and associated parameters such as phonon frequency, polarization, group velocity, and density-of-states) is obtained via the VFF approach available in the open source NEMO 3-D toolkit and compared with an empirically fitted model (against experimental data) as provided by Brockhouse [3].

$$\omega = 9280 \bullet K - 2.234 \times 10^{-7} \bullet K^2 \text{ [LA]}$$

$$\omega = 5240 \bullet K - 2.278 \times 10^{-7} \bullet K^2 \text{ [TA]}$$

On the other hand, the MC transport kernel is built upon 3 (three) discretization schemas, namely, 1) *Spatial*: the geometric volume is divided into multiple cubically stacked spatial bins/cells; 2) *Temporal*: to track the phonon drift in time; and 3) *Spectral* (frequency). After initializing the phonon ensembles and defining their properties (via the use of various probability distribution functions and random numbers), the ensembles are allowed to drift from their respective position towards the colder end using an explicit 1st-order time integration equation. As the ensembles drift inside the nanostructure, they interact with the structural boundaries, atomic impurities and other phonons.

RESULTS AND DISCUSSION

Fig. 2 shows the group velocity (v_g) profiles for a silicon film (thickness ~4 μm) obtained from the VFF and the empirical models. At this moment, VFF is used only for the LA (faster) branch. It is seen that the VFF computed v_g for the LA branch is smaller for $\omega < 5\times10^{13}$ rad/s and then increases for higher frequencies when compared to the empirical model. Fig. 3 shows the thermal conductivity profiles plotted using the atomistic VFF and the empirical approaches. Looking at the Figure it is found that, as compared to the empirically fitted model, the thermal conductivity calculated using the VFF approach deviates by about 8% (~18 W/m-K) (due to the incorporation of atomistic corrections in the LA branch alone). The VFF-MC approach, used in this work, not only allows one to capture the atomicity of the lattice but also enables the simulation of realistically sized structures containing millions of atoms. A corrected VFF (for the TA branch) and how the results obtained from the VFF-MC framework are used in the multiscale modeling of thermoelectric cooler units will be the subjects of future study and presented at the Workshop.

*Supported by NSF Grant No. 1218839.

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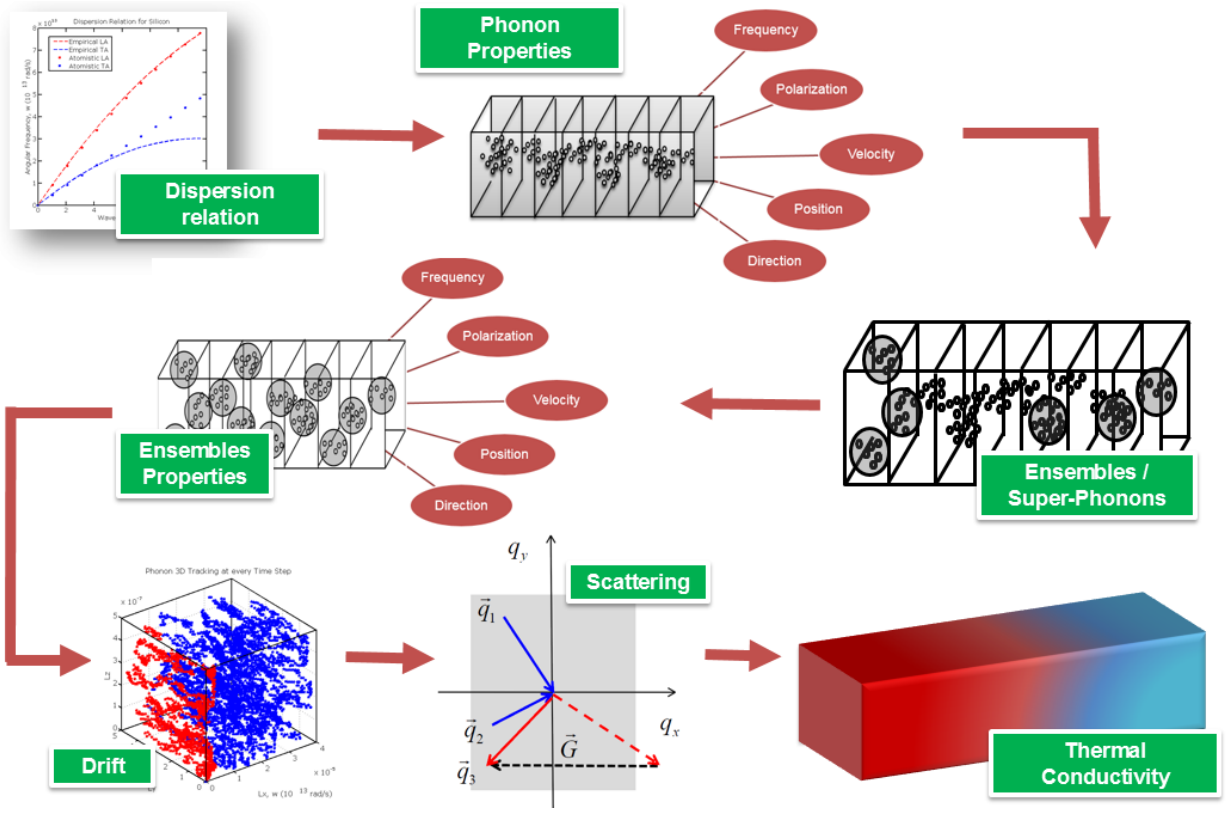

Fig. 1. A high level flowchart showing various steps/modules involved in the MC scheme.

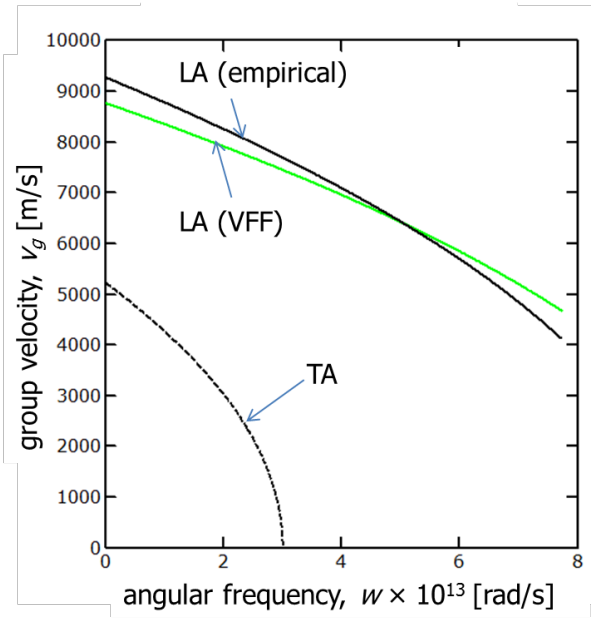

Fig. 2. Phonon group velocity profiles in silicon thin film of thickness ~4 μm using the VFF and the empirical approaches.

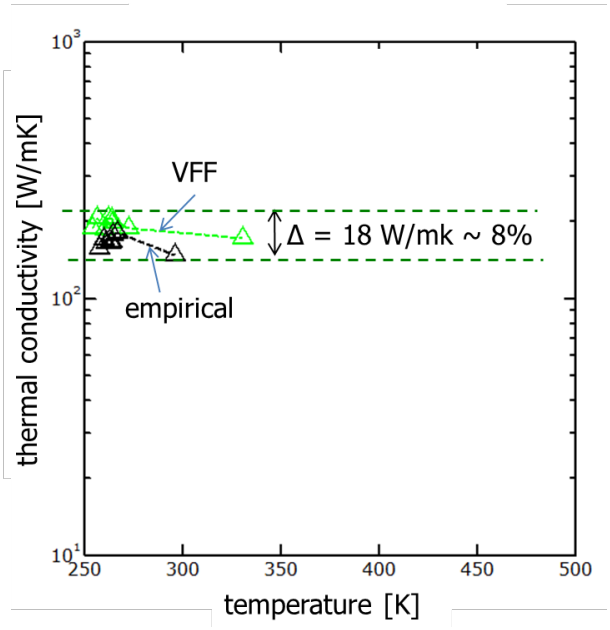

Fig. 3. Thermal conductivity computed using the VFF and the empirical approaches.