Full Band Monte Carlo simulation of transient and stationary thermal transport in GaAs porous nanostructures based on *ab initio* calculation

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INTRODUCTION

Semiconducting materials such as GaAs are a key technology for increasing the energy efficiency of electronic devices [1]. Despite significant progress in thermal transport modeling beyond Fourier's law, the analysis of the nanostructures with porous that fully capture their properties are still scarce [2].

In this work, we present a full-band Monte Carlo (MC) approach based on the Boltzmann's transport equation (BTE) for phonons using ab initio parameters. Thermal conductivity, transient and stationary properties of GaAs nanostructures are analyzed in all phonon transport regimes.

METHOD

All necessary material parameters including scattering rates are calculated by ab initio methods in the framework of the density functional theory (DFT) as implemented in Quantum ESPRESSO [3], as shown in Fig. 1.

To solve the BTE that describes the time evolution of the phonon distribution function, our home-made Monte Carlo simulator is used and detailed implementations are presented in [4]. In Fig. 2 investigated nanowires and nanofilms in both cross-plane and in-plane configurations are shown. Nanowires have only diffusive external boundaries that randomize the propagation direction of reflected phonons. To mimic the effect of nanopores in the simulated device, the boundaries of each nanopore are assumed to be diffusive.

RESULTS

We first investigate the dependence of thermal conductivity on the length, temperature and porosity in cross-plane nanofilms (CPNF). Our simulation results are compared to semi-analytical models and experimental data in Fig. 3. The phonon transport gradually changes from a ballistic regime in ultra-short films to a diffusive one in long nanofilms, and thermal conductivity decreases depending on the porosity due to the degradation effect of nanopores. Figure 4 shows that the conductivity reduction is directly related to the number of rough boundaries when the heat transport is diffusive. The ratio of thermal conductivity of CPNF calculated by MC simulation to semi-analytical ballistic one is plotted in Fig. 5 (a) showing the degree of ballisticity of transport. The transient thermal response is investigated by analyzing the time evolution of heat flux density at different positions as shown in Fig. 5 (b). Finally, Fig. 6 shows the spectral contributions of the thermal flux for each device of different length. Optical phonons can contribute over 20% to thermal conductivity in ultra-short devices where ballistic transport dominates.

CONCLUSION

We have proposed a stochastic Monte Carlo algorithm parameterized with *ab initio* calculations efficient for predicting the thermal properties of diverse nanostructures at all time and dimension scales.

ACKNOWLEDGMENT

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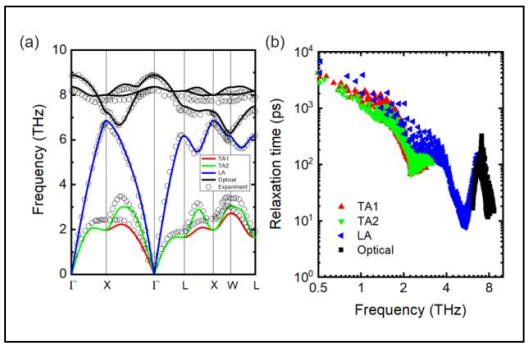

Fig. 1. (a) Calculated phonon dispersions for GaAs along the high symmetry paths and experiment data [5]. (b) Phonon relaxation times as a function of frequency at 300 K for different modes computed via DFPT.

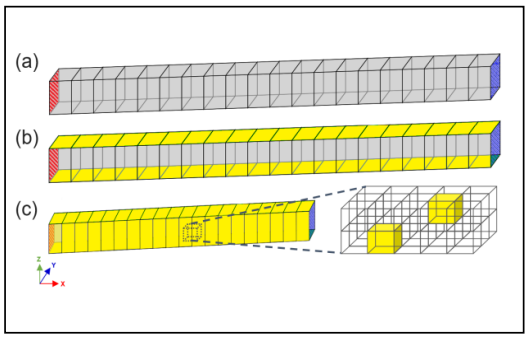

Fig. 2. (a) Nanofilm in cross-plane configuration (CPNF), (b) Nanofilm in in-plane configuration (IPNF), (c) Nanowire (NW) and partial diffusive internal structure for mimicking nanopores. Red/blue faces for hot/cold thermostats T_H=302K, T_C=298K, respectively. Yellow faces for diffusive boundaries.

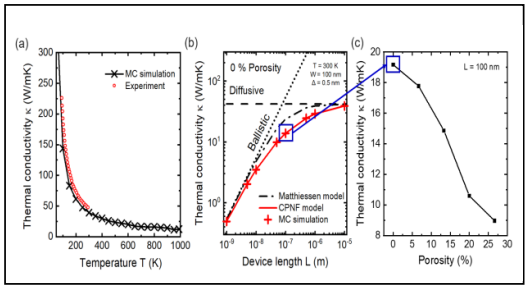

Fig. 3. (a) A comparison between the thermal conductivity of MC simulation results and experiment data [6]. (b) Thermal conductivity as a function of length and (c) the effect of nanopore density for CPNF.

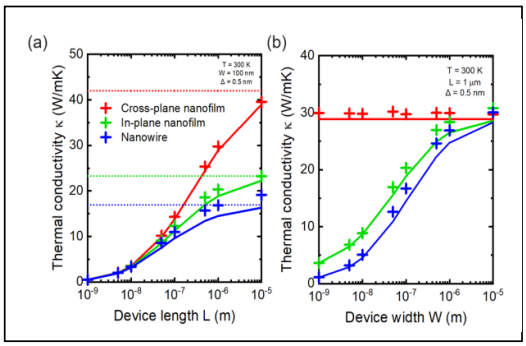

Fig. 4. Thermal conductivity κ as a function of (a) length L with 100 nm width and (b) width W with 1 μm length for CP and IP nanofilms and for nanowires at 300 K. Solid and dotted lines represent for semi-analytical models and long-device thermal conductivity, respectively.

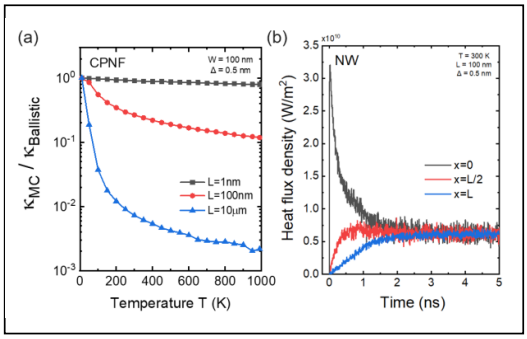

Fig. 5. (a) The Knudsen number calculated by MC simulation as a function of temperature for CPNF with three different device lengths. (b) Heat flux density as a function of time for NW of length 100 nm at three different positions along the x-axis.

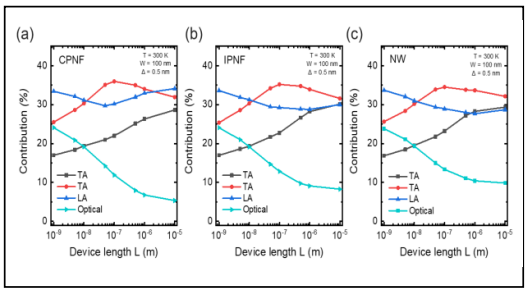

Fig. 6. Spectral contributions of each phonon mode to the total heat flux as a function of length for (a) CPNF, (b) IPNF, and (c) NW at 300 K.