Phonon transport in silicon nanowires using a Full-Band Monte Carlo approach

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INTRODUCTION

The miniaturization of electronic devices makes the thermal management in circuits a critical issue. At the nanometer scale, the heat transport is inaccurately modeled within the standard Fourier formalism. Indeed, the specific behavior of each phonon mode must be considered and the out-of-equilibrium nature of phonon transport becomes significant. In this context, we have developed a new Full Band (FB) Monte Carlo (MC) code dedicated to the phonon transport to investigate the thermal effects in silicon nanowires. In this code, the phonon dispersion is computed over the whole Brillouin zone using the atomistic Adiabatic Bond Charge Model (ABCM).

MODEL AND RESULTS

The semi-empirical ABCM method is kown to compute accurately the phonon mode dispersions in silicon lattice (Fig. 1.a) [1,2]. In this approach, charged particles, called Bond Charges (BCs), are introduced between positive atomic ions to mimic the electron shell and assure the total electrical neutrality. As schematized in Fig 1.b and within an adiabatic assumption for the BCs displacements, four forces are involved in this model, including the Coulomb force. Finally, only four empirical parameters are needed.

In Fig. 2, phonon dispersions obtained from our ABCM calculation along [110] are compared with those of the widely used analytical isotropic quadratic fit [3]. As this fit has been made along [100] direction, the analytical dispersion is far from experimental values along [110]. In contrast, the ABCM values reproduce very well the experimental data over the whole Brillouin zone. Similar limitation of the analytical model is observed on the specific heat at room temperature plotted in Fig. 3.

To simulate the phonon transport in silicon bars, a full-band MC approach has been implemented. As summarized in Fig. 4 in the first step of the MC algorithm, the initial position and the wave vectors of each simulated phonon are randomly selected. During each time step, some phonons are injected in through thermal contacts and the phonons already in the device undergo a series of free flights and scattering processes. The scattering mechanisms are implemented within the relaxation time approximation according to the approach proposed in Ref. [4].

The energy spectrum of phonons after the initialization step is plotted in Fig. 5. It reproduces well the theoretical spectrum obtained by multiplying the ABCM Density Of State (DOS) and the Bose-Einstein distribution. The evolution of the thermal conductivity in Si within an analytical description of the band structure calculated via the MC simulator is shown in Fig. 6.

In the next step, the evolution of the phonon flux in nanowires as a function of the temperature bias will be investigated. The size effect: quantum confinement and out of equilibrium transport related respectively to the transverse and the longitudinal direction will be carefully examined.

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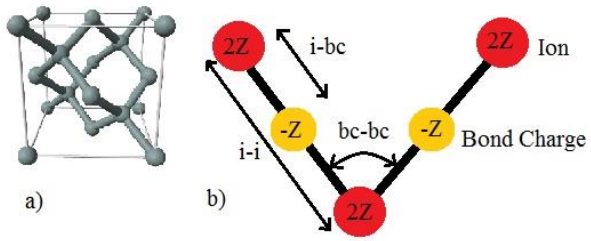

Fig. 1. a) Unit cell of silicon. b) Forces between the silicon ions and the bond charges in the ABCM. i-i and i-bc are bond-stretching forces. Bc-bc is a bond-bending force. Z is an electric charge which induces electrostatic forces.

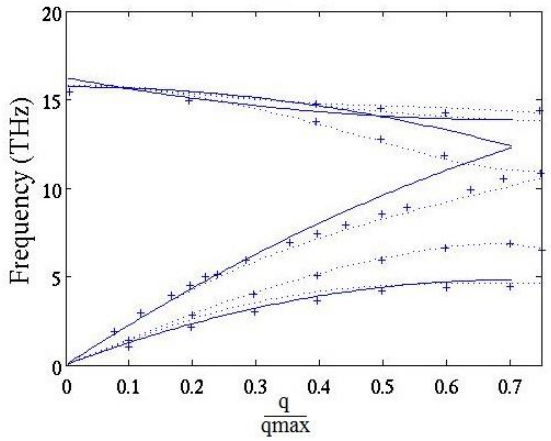

Fig. 2. Phonon dispersion along the direction [110] in silicon. The wave vector is [q,q,0] and $qmax$=2π/a where a is the lattice parameter. The experimental values (crosses) are from ref. [1]. Dashed lines show the ABCM results. Solid lines represent the quadratic isotropic fit along [100].

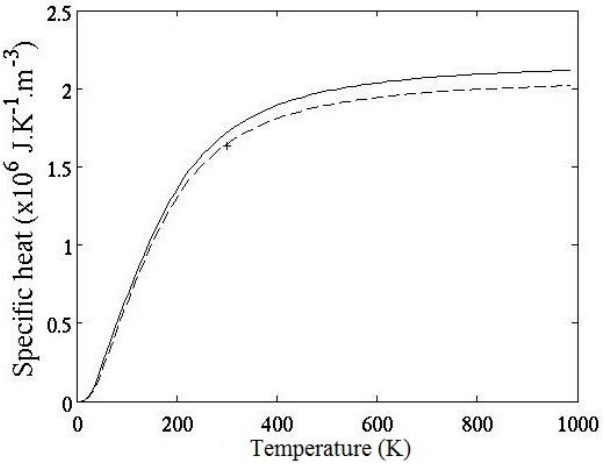

Fig. 3. The dashed (solid) line is the specific heat computed within the dispersion from the ABCM (analytical dispersion). The cross symbol reports an experimental value from [5].

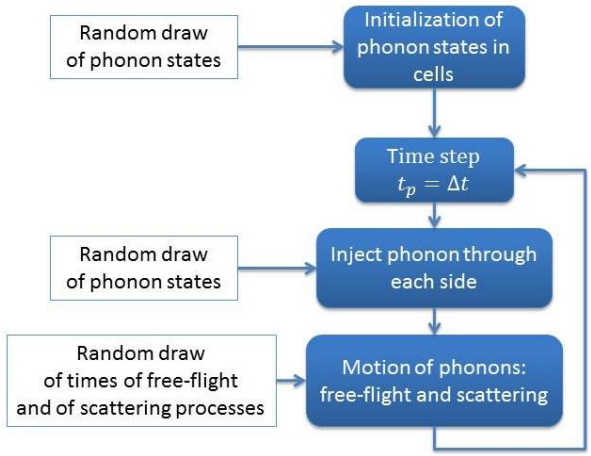

Fig. 4. Monte Carlo algorithm dedicated to phonon transport.

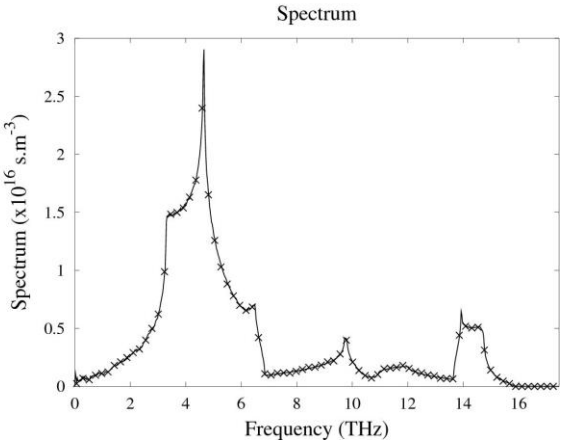

Fig. 5. The crosses are the data of the spectrum of phonons randomly selected by our algorithm for a silicon bar at 300 K. The solid line is the theoretical spectrum at 300 K.

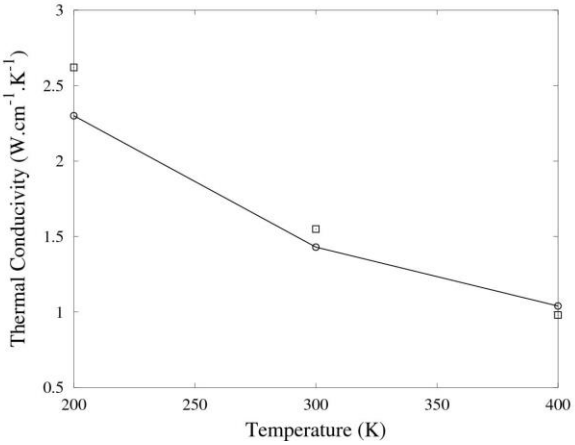

Fig. 6. The circles are the thermal conductivity of bulk silicon computed via the Monte Carlo algorithm using an analytical dispersion. Squares are experimental data from [5].