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Thermal Conductivity of Silicon Nanowire Using Nonequilibrium Molecular Dynamics Simulation

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Abstract
In this paper, nonequilibrium molecular dynamics for computing the thermal conductivity of two silicon nanowires (SiNWs) with different cross sections; circular and rectangular has been used. Diameter of the circular case is 22nm. The thermal conductivity of individual single crystalline SiNW with diameter of 22nm and total number of 2281825 Si atoms was computed, so we were able to compare our results with previous experimental reports. We used Sillinger-Weber silicon as our model system. Then, we considered SiNW size effect on the thermal conductivity and used extrapolation to compute the thermal conductivity of an infinite length SiNW. In the other approach of this paper, we compared the thermal conductivity of straight and corrugated SiNWs with rectangular cross sections to see the effects of corrugation on the thermal conductivity. It is obvious that, the thermal conductivity of the SiNW will decreases by increasing the size of the corrugation. According to the strong phonon scattering at the free surface of SiNW, the computed thermal conductivity was lower than its bulk value.

Keywords: Molecular Dynamics; Silicon Nanowire; Thermal conductivity

Introduction

Semiconductor fabrication technology has been developed rapidly and nanowires are getting much attention as the result of their applications in microelectronics, optoelectronics, and energy conversion devices. The electrical conductivity of a semiconductor material increases with increasing temperature, which is behaviour opposite to that of a metal. Semiconductor devices can display a range of useful properties such as passing current more easily in one direction than the other, showing variable resistance, and sensitivity to light or heat. Predicting the nanowires thermal conductivities is very important in making these devices. So, the heat treatment consideration of nanowires has received noteworthy research interest. In addition, a deeper understanding of thermal transport in nanostructures also has practical implications [1] in the design and performance of modern microelectronic devices that have sub-100 nm features and recently proposed nanowire-based thermoelectric devices

Molecular dynamics simulations [2] have shown that, for wires of nanometer diameter, the thermal conductivities could be two orders of magnitude smaller than that of bulk silicon. It is, therefore, important to experimentally validate these theoretical predictions to understand the underlying physics. Experimental results of the thermal conductivities of SiNWs by Li et al showed that SiNWs thermal conductivities are two orders of magnitude lower than their bulk value and among four samples with diameters of 22, 37, 56 and 115 nm, the thermal conductivity of the 22 nm nanowire has the most obvious size effect [3].
Molecular dynamics (MD) is a powerful tool which has been recently developed to study the thermal properties of nanostructures. In this research, nonequilibrium MD simulations are used to calculate the thermal conductivity of a SiNW with diameter of 22nm and with 30 to 120 nm lengths. We also compute the thermal conductivity of corrugated SiNW with rectangular cross section area. Results are compared with experimental values and the differences will be discussed.

Simulation Method

The schematic figure of circular and rectangular SiNW is shown in Fig.1 and Fig. 2, respectively. The silicon crystalline could be modeled using a many body potential function like Stillinger-Weber **(**SW**)** potential for describing the atomic interactions.
Equations of motions are integrated with velocity Verlet algorithm with a time step of $\Delta t=5fs$. Fixed boundary conditions are exerted along the length direction by freezing two ends of the system. Nose-Hoover thermostat is applied about *300ps* to equilibrate and relax the system. By rescaling atomic velocities at each time step, a known amount of kinetic energy $\Delta\varepsilon$ is added into the hot region and subtracted from the cold region. When the system reaches to steady state, the heat flux can be calculated by:

$$j=\Delta\varepsilon/(A\Delta t) \quad (1)$$

where A is the cross-section area.
In all simulations the local temperature T is also averaged over a million time steps. The temperature gradient could be used to obtain κ from Fourier's law $j=-\kappa\nabla T$. The temperature gradient and $\Delta\varepsilon$ vs. Δt for SiNW with L=120nm is shown in Fig.3 and Fig.4,