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 Stillinger-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 $\Delta E$ 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:

$$j=\Delta E/(A\Delta t)$$

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 $\kappa$ from Fourier's law $j=-k\nabla T$. The temperature gradient and $\Delta E$ vs. $\Delta t$ for SiNW with L=120nm is shown in Fig.3 and Fig.4,

ICHMT2014, 19-20 November, 2014
Results and Discussion

In this section, we present and discuss about the computed thermal conductivity of the SiNWs. The considered lengths of circular SiNWs are 30, 60, 90, and 120nm, respectively. According to the computing limitations, we are not able to investigate longer nanowires. Computed results are shown in figures 3 to 5. At room temperature, the mean free path of a crystalline silicon NW is around 300nm which is longer than our studied length of NW, so the thermal conductivities of our simulated samples are smaller than the bulk value. Schelling proposed that, for eliminating the finite size effects, we can find the thermal conductivity of an infinite NW by extrapolating the reciprocal of thermal conductivities vs. reciprocal of length [4] as shown in Fig.5. Using this method gives the value of 57.14 W/mK for the thermal conductivity of a silicon NW with diameter 22nm in MD temperature 300K without any quantum correction. Since the temperature 300K is under the Si Debye temperature, we should do some quantum corrections on our results. So according to Wang et al [5] reports, the real temperature would be about 200K and we should multiple the MD thermal conductivity to a factor of 0.66 to reach to the quantum corrected thermal conductivity which will be equal to 37.71 W/mK.

However, this value is still far away from empirical reports. The reason might be due to the rough surface of the synthesized NW in the experiment, while the simulated NW has a smooth surface and consequently longer phonon mean free path.

In order to investigate the effect of corrugation on the thermal conductivity of SiNW, we simulate rectangular SiNWs with three different corrugation height (h) as following:

1) Straight SiNW (h=0): Fig.6 and Fig.7 show the temperature distribution and energy flux for straight SiNW with zero corrugation height. The calculated
thermal conductivity is 5.91 W/m.K for this case.

2) Corrugated SiNW (h=2nm): Fig.8 and Fig.9 show the temperature distribution and energy flux of SiNW with corrugation h=2nm. The calculated thermal conductivity is 4 W/m.K for this case which is 32 percent lower than that of the straight case.

3) Corrugated SiNW (h=4nm): Fig.10 and Fig.11 show the temperature distribution and energy flux of SiNW with corrugation h=4nm. The calculated thermal conductivity is 1.13 W/m.K for this case which is 80 percent lower than that of straight case.

Conclusions

In this research, the thermal conductivity of a MD simulated silicon NW computed and compared with empirical result for diameter of 22nm. It was deduced that, the thermal conductivity of silicon NW significantly decreased compared to that of bulk Si. The low thermal conductivity of SiNWs makes them applicable in designing thermoelectric devices. As the second part of this paper we considered the effects of corrugation height of the SiNW over the thermal conductivity. It is obvious that, the corrugation has affected the thermal conductivity of the SiNW. As the values of the corrugation increases, the thermal conductivity decreases.


