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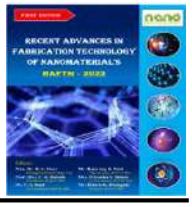

Temperature Domain Thermal Conductivity Engineering of One-Dimensional Silicon Square Nanowire

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KEYWORDS

Thermal Conductivity;
Dynamics Simulation;
1D Nanostructures,
Silicon Square Nanowire,
Nanoscale Nanomaterials.

ABSTRACT

For investigation of thermal conductivity in nanoscale nanomaterials, various experimental methods and theoretical predictions are considered. Nowadays, rising up of modelling and simulation is because it is a critical tool for researchers which allow optimizing designs without complications and the significant cost of nanofabrication processes. Thermal conductivity is a critical parameter to enhance the performance of thermoelectric devices. Silicon square nanowire (SiSqNw) is scalable thermoelectric material. Engineering thermal conductivity at nanoscale dimensions is more challenging. In this paper, the length of the simulation cell taken is 29.3618 nm and the empirical interatomic potential used for Si-Si interaction is Stillinger-Weber potential. Thermal conductivity of silicon square nanowire at temperature of 0.001K to 10,000K varied logarithmically is calculated by nonequilibrium molecular dynamics simulation (NEMD). At 300 K temperature, thermal conductivity of silicon square nanowire (SiSqNw) is 2.75451 W/mK. The dependence of novel properties of silicon square nanowire such as accumulative kinetic energy, average temperature, and thermal conductivity on temperature is studied.

1. Introduction

At nanoscale level and in real experiments which are difficult to perform, the molecular dynamics (MD) simulation is an alternative to predict the thermal conductivity, to unveil the mechanism and factors affecting heat conduction in nanowires [1]. The MD has become a valuable and promising tool in the field of thermal science and plays an important role in predicting thermophysical properties of materials from atomic/molecular viewpoint. Molecular dynamics simulation is used for solids within the classical limit which shows temperatures higher than the Debye temperature [2]. High thermal conductivity reduce device temperatures by removing heat to improve performance of nanoelectronics and optoelectronics, while low thermal conductivity is useful in thermoelectric for improving the figures of merit ZT of material.$ZT = S^2\sigma T/k$ Where S is Seebeck coefficient, σ is electronic conductivity, T is temperature, k is thermal conductivity [3]. Thermal conductivity is utmost important thermophysical property for thermal management and thermoelectric applications[4].

Low thermal conductivity is of particular interest in thermoelectric applications [5].The efficiency of thermoelectric devices depends upon the thermal conductivity which converts heat energy to electricity [6] Because of a higher surface to volume ratio, a significant reduction of the thermal conductivity is observed in nanowires [7]. The thermal conductivity of silicon nanowires is about two orders of magnitude smaller than that of bulk crystals due to the strong surface inelastic scatterings [8].Nonequilibrium molecular dynamics simulation is based on Fourier law of heat conduction which expresses thermal conductivity as the ratio of heat flux to temperature gradient [4].

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Semiconducting silicon nanowires attracted great attention in recent years due to their excellent electrical and mechanical properties and potential applications in many areas solar cell [9], field effect transistors[10], lithium ion batteries. Thermal conductivity of SiSqNw within a temperature domain of 0.001K to 10,000K is not studied yet. So, the present work investigates the thermal conductivities of SiSqNw at different excitation temperature.

This study also investigates the dependence of thermal properties of SiSqNw on a) time domain accumulative kinetic energy at different temperature; (b) position domain average temperature at different excitation temperature; (c)time domain average temperature in the silicon square nanowire at different excitation temperature;(d) time domain kinetic energy at different temperature; (e) kinetic energy dependent thermal conductivity of the silicon square nanowire; (f) temperature dependent thermal conductivity of the silicon square nanowire.

2. Methodology

By using Stillinger-Weber inter atomic potential [11] model for Silicon and Nonequilibrium molecular dynamics simulation, time dependent positions $r_i(t)$ of silicon nanowire and velocities $v_i(t)$ of the nanowire atoms are calculated.

The Thermal conductivity is calculated using heat flux J to form temperature gradient.The heat flux J continuously transfer energy from hot bath to cold bath[12]

$$J = \frac{\sum_{N\ transfer} \frac{1}{2}(m_h v_h^2 - m_c v_c^2)}{t\ transfer} \qquad (1)$$

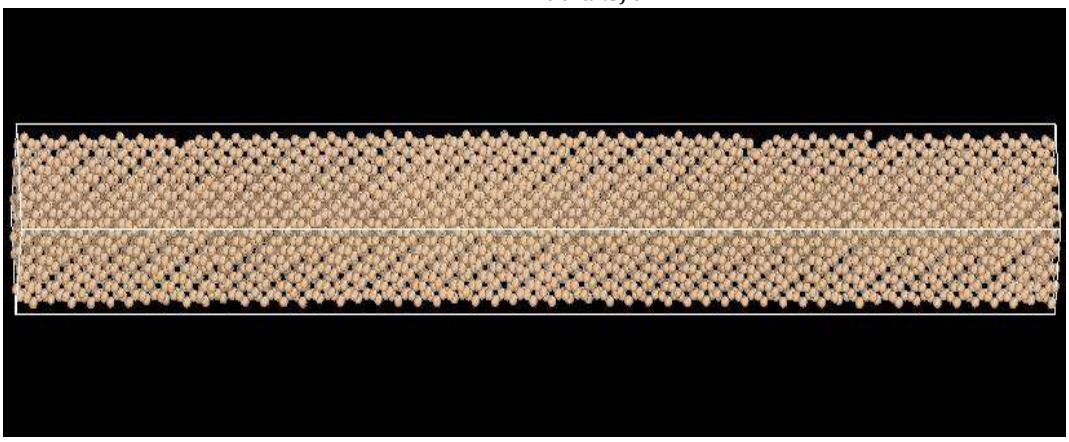

Fig.1 Silicon square nanowire directed along z direction

The heat flux is imposed by a velocity swapping technique. Atoms with the largest K.E. (i.e. hottest) in the heat sink are exchanged with those with lowest K.E.(i.e., Coolest in the heat source).The simulation cell is divided into even number of bins. The temperature of each bin and its temperature gradient is calculated by averaging the atomic K.E. over time as well as overall the atoms in the bin. The temperature$T_{MD}(z)$of a bin along the z-direction (i.e.the direction of heat flux) at every time step is determined from statistical mechanics equipartition theorem as

$$T_{MD(z)} = \frac{1}{3n_K k_B} \sum_{i=1}^{n_k} m_i v_i^2 \qquad (2)$$

Where k_B is the Boltzmann constant,n_k is the number of atoms in the bins about z and m_i and v_i are the mass and velocity of individual atoms i respectively [13].Position domain average temperature at different excitation temperature is used to calculate temperature gradient $\frac{\partial T}{\partial x}$ .Thermal conductivity λ is calculated by Fouriers law

$$\lambda = \frac{J}{2A\frac{\partial T}{\partial x}} \qquad (6)$$

Where, J is heat flux and $\frac{\partial T}{\partial x}$ is temperature gradient.

3. Simulation Set Up

For this NEMD simulation, silicon square nanowire is orientated along the z [001] direction. In NEMD method the simulation cell length in the transport direction is supposed to be sample length as in real experiment [14]. Here periodic boundary condition is along z direction and free boundary condition is along X and Y directions. In this study, the length of the simulation cells is 29.3618 nm. The cell parameter of Si is 0.543737037nm.Along the transport direction, simulation cell has 24 bins of silicon material. To calculate thermal conductivity, simulation cell is divided into 24 bins along z [001] axis. The cross-sectional area of the simulation cell is (5 x 5 x 54-unit cells) which gives 10800 atoms. The effective size of transport is14.6809 nm. Hot and cold heat baths have 3 bins. Non-equilibrium molecular dynamics (NEMD) simulations is performed using inhouse code via Nano-HUB [15]. For the thermalization run, the initial temperature of the system is 300 K and thermalization has been done for 10,000 MD steps, which equilibrate the system to the desired temperature. The time for MD is 2 *fs.* Next temperature ranges from 0.001K to 10,000 K is applied to both heat baths. The temperature of the heat bath is maintained at particular temperature for every cycle of the simulation through re-scaling the velocity of the atoms in that region to fit the Boltzmann distribution for the specific temperature. Interatomic potential used is Stillinger-Weber potential and 40,000 MD time steps are used to run simulation. First 20,000-time steps are used to achieve steady state of the heat transport and remaining 20,000-time steps are used to run thermal conductivity calculations.

4. Results and Discussions

Figure 2 depicts the simulated atomic trajectories of SiSqNw is visualized within excited temperature range with the help of OVITO [16]. From Atomic trajectories, It can be seen that as temperature increases atoms of SiSqNw are disordered more with respect to earlier one.At 10000K atoms of SiSqNw crosses it's own boundary.

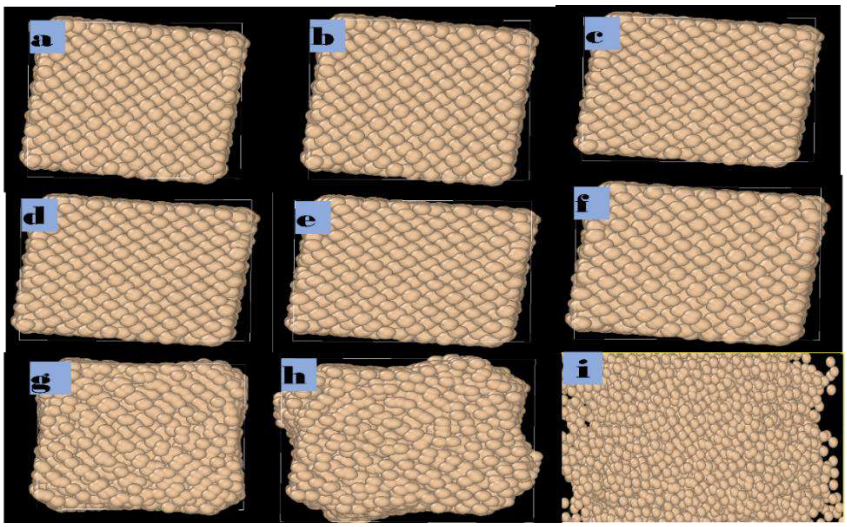

Fig. 2 Atomic trajectories of SiSqNw at temperature of a)0.001K, b)0.01K, c)0.1K, d)1K, e)10K, f)100K, g)300K, h)1000K, i)10000K

In order to validate the computational model of SiSqNw the simulation is carried out and shown in Fig. 3. The accumulative kinetic energy is found to be low at lower temperature and found to be increased at higher temperature. Furthermore, sudden change in the accumulative kinetic energy is observed for all scanned temperature range and become saturated after some time. The average temperature in units of Kelvin versus position in units of angstrom is plotted at differing temperature ranges from 0.001K to 10000K for the simulated system. At the cold bin and Hot bin, the temperature is nonlinear due to size effect [17]. In order to avoid edge effect, middle linear portion has been used to extract temperature gradient for the determination of thermal conductivity using following equation $\boldsymbol{\lambda} =$

$\frac{J}{2A\partial T/\partial x}$. The factor 2 in the denominator is used to account for the periodicity of the system [18]. The average temperature in units of Kelvin versus time in units of picoseconds at different temperature range of 0.001K to 10000K are calculated for system. The linear behavior is observed at higher temperature whereas non-linear behavior is observed at lower temperature. The kinetic energy in units of Kcal/mol versus time in units of picoseconds is plotted at different excitation temperature.From the simulation, it is observed that the thermal conductivity of material is decreased as the kinetic energy is increased. Further increase in the kinetic energy, a sudden increase in the thermal conductivity is observed. In addition to this the thermal conductivity is found to decrease at higher kinetic energy.Thermal conductivity is found to decrease with increase in temperature upto 1K and again thermal conductivity rises upto 300K.From 300K temperature,thermal conductivity decreases upto 10,000K temperature. This is due to the fact that at low temperature,k is proportional to T^3 while phonon mean free path is constant. Above 300K, thermal conductivity starts to decline. This is because heat capacity is constant at high temperatures whereas thermal conductivity is inversely proportional to temperature.

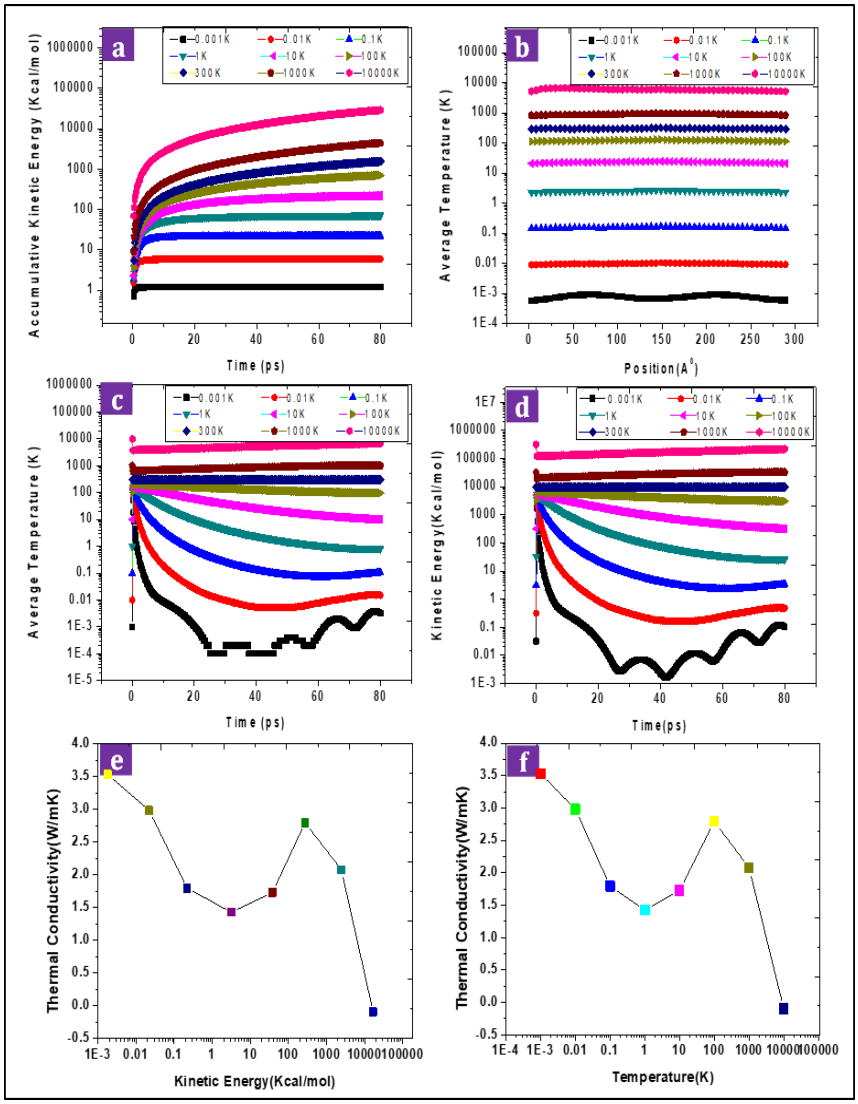

Fig. 3: Thermal properties of Silicon Square Nanowire. (a) time domain accumulative kinetic energy at different temperature; (b) Position domain average temperature at different excitation temperature; (c) Time domain average temperature in the Silicon Square Nanowire at different excitation temperature;(d) time domain kinetic energy at different temperature; (e) kinetic energy dependent thermal conductivity of the Silicon Square Nanowire; (f) temperature dependent thermal conductivity of the Silicon Square Nanowire.

5. Conclusions

In this chapter, non-equilibrium molecular dynamics simulations are performed to explore the thermal conductivity engineering of SiSqNw at a temperature range of 0.01K to 10000K.The thermal conductivity of silicon square nanowire increases with rise in temperature from 1K upto 300K and then considerably decreases. This is due to the fact that at low temperature,k is proportional to T^3 while phonon mean free path is constant. Above 300K, thermal conductivity starts to decline. This is because heat capacity is constant at high temperatures whereas thermal conductivity is inversely proportional to temperature. At 300 K temperature, thermal conductivity of SiSqNw is 2.75451 W/mK. Low thermal conductivity is useful for researchers in thermoelectric applications. This chapter paves the way to better understand thermal management.

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