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Effects of vacancy defects and axial strain on thermal conductivity of silicon nanowires: A reverse nonequilibrium molecular dynamics simulation

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ABSTRACT

Thermal conductivity of silicon nanowires (SiNWs) is evaluated using the reverse nonequilibrium molecular dynamics simulation. The Stillinger–Weber (SW) and Tersoff interatomic potentials are employed to simulate thermal conductivity of SiNWs. In this work, the influence of random vacancy defects, axial strain, temperature and length on thermal conductivity and effective mean free path of SiNWs is investigated. It is found that by raising the percent of random vacancy defects, thermal conductivity of SiNWs decreases linearly for the results obtained form SW potential and nonlinearly for those obtained from Tersoff interatomic potential. Dependence of the thermal conductivity on axial strain is also studied. Results show that thermal conductivity increases as compressive strain increases and decreases as tensile strain increases. Influence of temperature is also predicted. It is found that the thermal conductivity of SiNWs decreases with increasing the mean temperature. Most of the simulations are performed for 4 UC × 4 UC × 40 UC silicon nanowires using ssp boundary condition.

1. Introduction

Silicon nanostructures are extremely regarded during last years for their new physical and chemical characteristics. Among the silicon nanostructures, silicon nanowires (SiNWs) are highly considered due to their thermoelectric, optical, electrical and thermal properties and a great deal of researches have been focused on fabrication, investigation and applications of these nanostructures. It is shown that silicon nanowire field effect transistors (SiNWFETs) [1–3] can be a reliable candid for biosensors which they are real-time, high selective and high sensitive [4–6]. They are also a nice choice for advanced energy storage and conversion devices [7] such as lithium-ion rechargeable batteries [8–10], photovoltaic devices [11–13], and thermoelectric devices [14–16]. Thermoelectric devices can convert heat (even waste heat) into electricity and vice versa and so they can be used for heating or cooling or for power generation. These generators have many advantages such as low pollution and long operating lifetime. Because of these advantages, many attempts have been made to improve the efficiency of thermoelectric devices. Results show that one dimensional (1D) nanostructured materials such as SiNWs have enhanced thermoelectric performance in comparison with the bulk materials [17]. In thermoelectric devices, lowering thermal conductivity without reducing electrical conductivity is desirable to improve the efficiency of thermoelectric energy conversion, and SiNWs is a promising candidate to achieve this goal [18–20]. Thermal conductivity of SiNWs can be affected by many of geometrical or physical factors such as their lateral dimension and length, defects, strain, temperature and etc. Unwanted structural defects which are generated during growing process may cause some changes in thermal conductivity of nanostructures. On the other hand, one can modify the thermal conductivity by adding defects or impurities for special purposes. This can enhance thermal transport in some devices based on nanostructures such as nano/microelectrical chips or improve efficiency of thermoelectric conversion. Besides some experimental attempts [21–23], theoretical modeling performs a significant role to predict the thermal conductivity of bulk silicon and also silicon nanostructures containing vacancies [24–29], impurities [30–32] and grain boundaries [33,34].

Wang et al. [29] studied the influence of lattice defects on the thermal conductivity of bulk silicon using nonequilibrium molecular dynamics method (NEMD). Their simulations reveal that the phonon relaxation time is the most important parameter to describe decreasing of thermal transport behavior in the defective structures.

Yaping and Galli [35] designed nanowires with a tailored surface structure and composition and specific core defects to

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investigate the microscopic origin of the reduced thermal conductivity of Si at the nanoscale. They found that combination of core defects and surface ripples decrease the magnitude of thermal conductivity.

Yamamoto et al. [24] studied the effect of vacancy defects on thermal conduction of SiNWs using nonequilibrium Green′s function approach. They found that the defects, reduce the thermal conductance significantly and the "center-defects" reduce thermal conductance much more than "surface defects".

Strain is another important factor which can effect on electrical, optical and mechanical properties of materials. Nano/microscale devices contain residual strain after fabrication. On the other hand in practical condition, materials and devices are almost under external compressive or tensile strain.Many attempts have been done to study the thermal conductivity of nanostructures under strain using experiments [36–39] and molecular dynamics simulations [40–43].

Ross et al. [42] concluded that the thermal conductivity of semiconductors increases with compressive strain. They explained that the phonon velocity increasesunder pressure and results in thermal conductivity enhancement.

It is indicated that for simple nanoscale strained heterostructures containing a single interface, the effective thermal conductivity may be less than the half value of the average value of the thermal conductivity of the respective unstrained thin films [43].

Li et al. [40] performed the equilibrium molecular dynamics simulation to study the strain effects on the lattice thermal conductivity of low-dimensional silicon and carbon materials. The thermal conductivity of the strained silicon and diamond nanowires and thin films was shown to decrease continuously when the strain changes from compressive to tensile.

The other effective factors on thermal conductivity are length, cross-sectional area and temperature [44–46]. The dependence of the thermal conductivity on the wire length, cross-sectional area, and temperature was investigated [44] and results showed that thermal conductivity for very long wires decrease with increasing temperature from 200 to 500 K, which is the same tendency as for bulk silicon. Cruz et al. [46] calculated the thermal conductivity of silicon nanowires as a function of crosssection and length. They found that the thermal conductivity increases with increasing SiNWs length.

In this work influence of random vacancy defects, compressive/tensile strain, temperature and length on thermal conductivity of SiNWs are investigated using reverse nonequilibrium molecular dynamics simulation.

2. Simulation method

The contribution of electrons in the heat conduction of silicon is much smaller than phonons. Therefore, classical molecular dynamics method can be used to predict phonon thermal transport properties. Choosing of interatomic potential for silicon depends on the type of atomic structure and the properties to be investigated. The Stillinger–Weber (SW) interatomic potential is accurately describes silicon elastic properties, phonon dispersion curves, and thermal expansion coefficients. The SW potential consists of following two and three-body interaction terms respectively [47]:

$$\phi_2(r_{ij}) = \begin{cases} \varepsilon A\left[B\left(\frac{\sigma}{r_{ij}}\right)^p - \left(\frac{\sigma}{r_{ij}}\right)^q\right] e^{\sigma/(r_{ij}-\sigma r_c)} & (r_{ij} < \sigma r_c) \\ 0 & (r_{ij} \geq \sigma r_c) \end{cases} \quad (1)$$

$$\phi_3(r_{ij}, r_{ik}, \theta_{jik}) = \begin{cases} \varepsilon\lambda e^{\left[\gamma\sigma/(r_{ij}-\sigma r_c)+\gamma\sigma/(r_{ik}-\sigma r_c)\right]} \times \left(\cos\ \theta_{jik} + \frac{1}{3}\right)^2 & (r_{ij}, r_{ik} < \sigma r_c) \\ 0 & (r_{ij}, r_{ik} \geq \sigma r_c) \end{cases} \quad (2)$$

where A, B, p, q, γ, ε, λ. and σ . are materials parameters, r_{ij} is the distance between atoms i and j, θ_{jik} is the angle between r_{ij} and r_{ik}, and r_c is the cutoff radius. From the simple quantum mechanical rules, the bond strength is highly related to coordination number and unfortunately this subject is not considered in the SW potential. Therefore this potential may not proper for the cases such as defective or strained structures which coordination number deviates from its natural value. Because of this crucial role of bond order and its dependence on local geometry, the Tersoff interatomic potential was introduced as [48]

$$\phi_{ij} = f_c(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \quad (3)$$

where f_R is the two-body term and f_A includes three-body interactions.

Gre are two kinds of computational methods for studding thermal conductivity of nanomaterials called continuum and atomistic models. The first one is a method thatusing continuum models and kinetic theory such as Boltzmann transport equation (BTE). In the atomistic models the system are represented as a number of atomic sites connected by chemical bonds. One of the most important methodes of atomistic simulations is molecular dynamics method which genrally is employed in two different way to evaluate thermal cunductivity of systems. These two methodes are called direct nonequilibrium molecular damics (DNEMD) [49,50] and reversed nonequilibrium molecular dynamics (RNEMD) [51,52]. In DNEMD method, the temperature gradient is directly applied tthe structure and resulted heat flux is measured. This method needs a large value of temperature gradient and so the mean value of heat flux converges slowly due to large fluctuations. The slow converges of temperature and also heat flux takes a high computational cost which is about few tens of nanoseconds. In addition this method needs thermostat to achieve nonequilibrium thermodynamics steady state which takes more computational time. In reverse nonequilibrium MD method, the heat flux applied to the system and the resulted temperature gradient is measured. This method has the advantage that the quantity of heat flux is a known parameter and need not to be calculated. Except this, the mean value of temperature gradient converges fast and takes only a few nanoseconds. Therefore this method has a much lower computational cost than direct method. Furthermore this method does not need thermostat due to conversation of energy and linear momentum. Because of these advantages RNEMD is employed in this work. In this method the simulation box is divided into N slabs along the heat transfer direction. Slabs 1 and $N+1$are defined as the cold slabs and the slab $N/2+1$ is defined as the hot slab. The slabs are chosen to be identical thickness and hence volume. Then in the specified time interval of the simulation, the hottest atom in the cold slab and coldest atom in hot slab are chosen and the velocity vectors of them are exchanged. By continuing velocity exchange, the temperature in the hot slab increases over the mean temperature and temperature in the cold slab decreases lower the mean temperature. This unphysical energy transport from cold slabs to hot slab causes a temperature difference between hot and cold slabs and soresults in a temperature gradient in the system. The heat flux due to this mechanism is given by [51]:

$$j_z = \frac{1}{2At}\sum_{transfers}\frac{m}{2}\left(v_{hot}^2 - v_{cold}^2\right) \quad (4)$$