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# Molecular dynamics study of the thermal expansion coefficient of silicon

Hossein Nejat Pishkenari *, Erfan Mohagheghian, Ali Rasouli

*Nano Robotics Laboratory, School of Mechanical Engineering, Sharif University of Technology, P.O. Box 11365-9465, Tehran, Iran*

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A B S T R A C T

Due to the growing applications of silicon in nano-scale systems, a molecular dynamics approach is employed to investigate thermal properties of silicon. Since simulation results rely upon interatomic potentials, thermal expansion coefficient (TEC) and lattice constant of bulk silicon have been obtained using different potentials (SW, Tersoff, MEAM, and EDIP) and results indicate that SW has a better agreement with the experimental observations. To investigate effect of size on TEC of silicon nanowires, further simulations are performed using SW potential. To this end, silicon nanowires of different sizes are examined and their TEC is calculated by averaging in different directions ([100], [110], [111], and [112]) and various temperatures. Results show that as the size increases, due to the decrease of the surface effects, TEC approaches its bulk value.





## 1. Introduction

Applications of nanostructures in nano- and microelectromechanical systems (NEMS and MEMS) [1–5] and microelectronic devices [6,7] have rapidly grown in recent years. Hence, predicting thermal properties of silicon, which is a common substrate for aforementioned systems, with sufficient accuracy, is crucial for almost all current and envisioned applications of nanostructured silicon. Design of a microelectronic device without a good knowledge of thermal properties of materials, may result in an unacceptable degree of curvature in the substrate, a prevalent problem which is called "wafer bow" [8–11]. In computational analysis of nano-scale structures, theories based on continuum assumptions cannot be directly applied to nanostructures [12]. Instead, when the size of materials becomes small, the surface and quantum effects as well as material defects play a significant role in the material properties.

Different methods for computational analysis of material properties are developed, each one being suitable for a certain type of problems. Generally speaking, the most accurate results are obtained using first-principles quantum-mechanical methods. The most significant disadvantage of these methods is their large computational cost for large systems [13]. To overcome this drawback, the computational cost must be reduced while maintaining a reasonable accuracy. This is accomplished by introducing empirical interatomic potentials [14–16]. The molecular dynamics (MD) method, which is based on interatomic potentials, is a powerful and convenient tool for predicting thermal properties of nanostructures. MD calculates the ensemble average of properties by gathering thermal statistics [17] and its results heavily rely upon the choice of the interatomic potential.

Many interatomic potentials have been introduced over the years. One of the most widely used potentials for silicon is Stillinger–Weber (SW). SW considers a linear combination of two- and three-body terms to express the cohesive energy [14]. Tersoff is another well-known potential which is proposed for covalent systems. In Tersoff, simple pairwise potential replaces the two- and three-body terms of interaction energy [15]. Also, Justu et al. developed environment-dependent interatomic potential (EDIP) and claimed partial improvements [18]. In MEAM (modified embedded atom method) potential, directional bonding is included and it can be applied to systems with covalent bonding [19].

Size and surface orientation effects on TEC of one-dimensional nanowires are also of interest. Experimental studies show that TEC of Cu and Bi nanowires are significantly lower than TEC of their bulk form [20,21]. Moreover, as size increases, TEC of nanowire approaches the bulk value. TEC is also dependent on the surface orientation with respect to the material crystalline direction; i.e. in different crystalline directions TEC may vary. These considerations play a vital role in designing silicon based nanoelectromechanical systems.

In recent years, MD simulations have been utilized to study thermal properties of materials [22–25] as well as their mechanical properties [26–30]. In particular, studies have been carried out to

* Corresponding author.
*E-mail address:* nejat@sharif.edu (H.N. Pishkenari).

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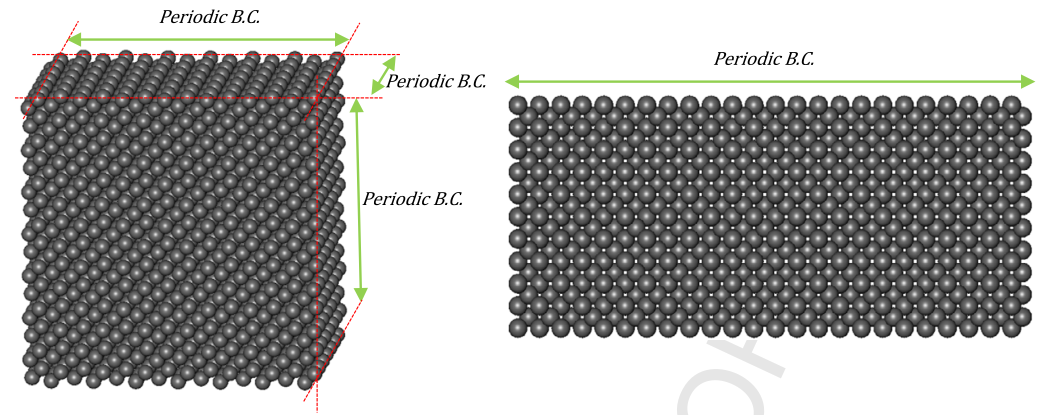


**Fig. 1.** Simulated samples of bulk (left) and nanowire (right) silicon.

study TEC of silicon [31–33]. Results obtained from all these simulations highly depend on the choice of the interatomic potential. In order to get satisfactory results, one should choose the potential based on the atomic structure of the system and the property under study [34]. Studies have been conducted to compare different empirical interatomic potentials [35–38]; however, to the best of our knowledge, no study has systematically compared potentials regarding thermal expansion coefficient of silicon. In this study SW, Tersoff, EDIP and MEAM are evaluated and TEC results are compared with experimental data obtained by Yim et al. [39] and Hiromichi et al. [40]. Based on the conducted simulations, the SW potential has the best agreement with the experimental observations amongst the four studied potentials. Then to examine effect of size on the thermal expansion coefficient of silicon nanowire, several simulations are conducted using SW potential.

In the following section, simulation setup is introduced. Afterwards, in section 3 results of different simulations are presented. Finally, in section 4 concluding remarks are made.

## 2. Simulation setup

In this research, MD simulations are conducted using LAMMPS solver [41]. Simulated samples are shown in Fig. 1. In the bulk model, periodic boundary conditions are applied along all three crystallographic directions. In the nanowire model, periodic boundary condition is only applied in the longitudinal direction. It is worth mentioning that the nanowire model has a square cross-section. Atomic interactions are described using Tersoff, SW, EDIP and MEAM, to figure out which potential has a better agreement with the experimental data. These potentials are the most recommended interatomic potentials for simulating silicon materials.

All simulations are performed with time step of 1 fs. To determine the optimal number of time steps, the average distance between two adjacent layers in the [100] direction is calculated. These calculations are carried out for silicon nanowire with dimensions of $6a \times 6a \times 15a$ in temperatures of 0.1, 500 and 1000 K. From the results, the optimal number of time steps is calculated to be 1.25 million for temperatures below 200 K, 2 to 3 million for temperatures between 200 and 500 K, and 3 million for temperatures over 500 K.

Initially, energy of the system is minimized and simulations are carried out in NPT ensemble to maintain the pressure and temperature of the system at a desired value during the run. Using NPT ensemble in MD simulations causes severe pressure fluctuations. To overcome this drawback, the optimal damping ratio of 600 is chosen and used in all proceeding simulations. In order to optimize the run time, effects of neighbor list and length of the nanowire are investigated. It is observed that the neighbor list of 2 and length of $8a$, where "$a$" is one lattice constant, save the computation cost without introducing any significant error.

For the calculation of the linear thermal expansion coefficient, 30 adjacent layers in the longitudinal direction of the nanowire are taken into account. The average distance between every two adjacent layers is calculated and then the linear thermal expansion coefficient is calculated using the following equation:

$$\alpha(T) = \frac{1}{\Delta T}\left(\frac{L_{final}(T) - L_{final}(T_0)}{L_{final}(T_0)}\right) \tag{1}$$

In this equation $\alpha(T)$ is the linear thermal expansion coefficient (TEC) while $L_{final}(T)$ and $L_{final}(T_0)$ are the average distances between 30 adjacent layers in the longitudinal direction in temperatures of $T$ and $T_0$ respectively. Throughout this study, $T_0$ is taken to be 273 K.

### 2.1. Quantum correction

Using classical molecular dynamics simulations, quantum effects are neglected which are noticeable at temperatures below the Debye temperature. In this regard, if we want to compare results of MD simulations with experimental data, we need to apply quantum correction to our MD results.

The accurate determination of quantum correction to the MD results is too intricate so we have employed a simple technique to apply quantum correction. In this technique, average temperature obtained by MD is simply rescaled to a temperature which includes the quantum effects. The reason for this rescaling is that the kinetic energy of our system at $T_{MD}$ is required to be the same as that of the corresponding quantum system at the scaled temperature, $T_{scaled}$ (including zero-point energy). Here, molecular dynamics temperature is rescaled according to the research done by Wang et al. [42] and all of our results are presented in the rescaled temperature unless specifically stated otherwise.

## 3. Results

Simulations are performed in two major parts. The first part investigates the effect of different interatomic potentials on the thermal expansion coefficient and lattice constant of bulk silicon. In the second part, effect of size is examined for nanowires using the potential that had a better agreement with experimental observations in the first part.

### 3.1. Effect of interatomic potential on TEC and lattice constant of bulk silicon

Considering the uncertainty in using different potentials, simulations are performed to investigate the effect of different po-



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