Atomistic Study on the Mechanical Behavior of Silicon-Base Nanotubes

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\textbf{Article Info} & \textbf{Abstract} \\
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\textit{Article history:} & Recently, silicon nanotubes (SiNTs) have been successfully synthesized and have attracted many researchers to work on the different aspects of them. In the present study, the stress-strain curve along with the Young’s modulus as a significant mechanical property of single walled silicon nanotubes at different diameters are determined. The simulation is performed by the use of molecular dynamics based on the Tersoff-Brenner many-body potential energy function. The results of the total strain energy of nanotubes as an accurate and effective methodology are used to establish appropriate expressions for evaluating Young’s modulus of the nanotubes. \\
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\textbf{Keyword:} & \\
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Mechanical behaviour & \\
Young’s modulus & \\
Molecular dynamics simulations & \\
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1. Introduction

The concept of ‘nanotechnology’ was proposed by physics Nobel laureate, Richard Feynman in 1959. Since then, nanotechnology has developed quickly and now is a significant technological advancement. Wide potential applications such as molecular electronics, diagnostic biosensors, and novel scanning microscopy probes \cite{1, 2}, make nanotubes one of the most popular nano filaments. In 1991, Iijima \cite{3} introduced carbon nanotubes. To study the mechanical behavior of nanostructure materials, molecular dynamics (MD) simulations are recognized as one of the most reliable techniques. Legoas et al. \cite{4} presented the first molecular dynamics simulation of carbon nanotubes as gigahertz oscillators. Researchers used MD simulations to investigate different aspects of carbon nanotubes and graphene, which are two phenomenal materials \cite{5-16}. Recently silicon nanotubes (SiNTs) have been successfully synthesized, and many authors have investigated different structures of SiNTs \cite{17}. Bahel and Ramakrishna \cite{18} calculated the lowest level of energy related to the possible structures of silicon nanotubes. Menon and Richter \cite{19} introduced a stable configuration of one-dimensional silicon. Fagan et al \cite{20} studied the stability and thermal behavior of SiNTs. Jahromi and Setoodeh \cite{21} investigated different vibration behavior of different SiNTs. The majority of the computer-aided studies and experimental results in open literature have been concerned with the basic mechanical properties of nanotubes under axial tension \cite{22, 23}. However, despite the wide potential applications of SiNTs, their mechanical properties are reported scarcely. This motivated the authors to study the tensile behavior of silicon nanotubes. Meanwhile, the Young’s modulus is determined for different diameters of Si nanotube for the first time. In order to obtain the more precise values of the modulus of elasticity, the total strain energy curve is employed.

2. Molecular dynamics simulation

Molecular dynamics is a powerful technique to explore the microcosmic mechanism of deformation and intrinsic characteristics of a structure at the atomic level. Also, it is a useful and reliable method to model the mechanical properties of nanostructures and nanomaterials. The basic steps of the molecular dynamics code include calculation of the interatomic forces, the elastic properties, the molecular bond energies, and the bond lengths of the Si-Si structure for each time step. Then Newton’s laws are used to determine the new positions and velocities from the old positions and velocities and the forces at each step. The present study pursues the Tersoff-Brenner many-body potential function to

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model the Si-Si interactions [24, 25]. The total potential energy for Si nanotubes based on Tersoff-Brenner potential is expressed as [26]:

$$\sum_i E_i = \frac{1}{2} \sum_{i \neq j} V_{ij}.$$  \hspace{1cm} (1)

With

$$V_{ij} = f_c(r_{ij}) [V_{rep}(r_{ij}) + b_{ij}V_{att}(r_{ij})].$$  \hspace{1cm} (2)

$$b_{ij} = b_{ij}(g_{ij}); \quad g_{ij} = \sum_k f_c(r_{ik})g(\theta_{ijk})f(r_{ij} - r_{ik}).$$ \hspace{1cm} (3)

where \(r_{ij}\) is the distance between pairs adjoining atoms \(i\) and \(j\), \(V_{ij}\) is the bonding energy, \(b_{ij}\) is an empirical bond-order term, \(V_{att}\) and \(V_{rep}\) are the attractive and repulsive parts of the potential, \(f_c(r_{ij})\) is the cutoff function and \(g_{ij}\) is a function in terms of coordinates [26]. In the present simulations, the Si-Si bond is equal to 2.245\AA\ [24], the canonical ensemble (NVT) at room temperature (300K) is considered and the boundary conditions in \(x\) and \(y\) directions are periodic. The nanotubes are extended axially (i.e. in the \(z\) direction), and the time step used in this model is 1 fs. The system is relaxed for 500 fs. The loading is applied to a set of atoms at the ends of nanotube in the form of displacement. This procedure is continued until the nanotubes take apart. The initial and deformed configurations of Si nanotubes are shown in Figure 1.

![Figure 1. Configurations of SINT in tensile, (a) unstrained; (b) strained; and (c) fractured condition.](image)

3. Results and Discussion

The molecular dynamics script Lammps is used in this work to develop the results. At first, the mechanical behavior of Si based nanotubes subjected to uniaxial tension is investigated. For instance, stress-strain curves for (10,10) and (5,5) silicon nanotubes are exhibited in Figure 2. Meanwhile, the Young’s modulus for each nanotube is determined using an accurate method by fitting a polynomial curve to the corresponding total strain energy data. Figure 3 presents the variation of the strain energy per atom which is determined by difference between the total energy per atom in strained and unstrained conditions with respect to the strain. Afterward, the Young’s modulus (\(Y\)) can be obtained from the second derivative of the total energy with respect to strain at the zero strain (i.e. at the equilibrium configuration) according to the following relation:

$$Y = \frac{1}{V_0} \left( \frac{\partial^2 E}{\partial \varepsilon^2} \right)_{\varepsilon=0}. \hspace{1cm} (4)$$

Where \(V_0\) denotes the equilibrium volume, \(\varepsilon\) is the strain and \(E\) stands for the total strain energy. There is an extreme challenge to determine the value of \(V_0\). Many researchers defined this volume using a shell-thickness equal to the interlayer spacing in graphene. Lammps molecular dynamics simulator’s data is another systematic procedure to evaluate \(V_0\) which is used here.
To validate the molecular dynamics simulation model the novel methods from Jahromi and Setoodeh are used to calculate the Young’s modulus of SiNT (10, 10) compared to their data in the literature as demonstrated in Table 1. The predicted value shows an excellent agreement with the solution of [21].

Table 1. Comparison of Young’s modulus of a (10, 10) SiNT

<table>
<thead>
<tr>
<th>Chirality</th>
<th>Y (GPa) Present</th>
<th>Y (GPa) Ref. [21]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10,10)</td>
<td>54.45</td>
<td>52.26</td>
</tr>
</tbody>
</table>

Table 2 illustrates the Young’s modulus of the silicon nanotubes with different diameters which were considered in the tensile test. It can be observed that the Young’s modulus forces a small variation with respect to the tube diameter.

Table 2. Young’s modulus of armchair SiNTs for different diameters.

<table>
<thead>
<tr>
<th>Chirality</th>
<th>Y (GPa) Present</th>
</tr>
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<tbody>
<tr>
<td>(5,5)</td>
<td>51.08</td>
</tr>
<tr>
<td>(6,6)</td>
<td>51.56</td>
</tr>
<tr>
<td>(7,7)</td>
<td>51.78</td>
</tr>
<tr>
<td>(8,8)</td>
<td>52.72</td>
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<tr>
<td>(9,9)</td>
<td>52.26</td>
</tr>
<tr>
<td>(10,10)</td>
<td>54.45</td>
</tr>
</tbody>
</table>

4. Conclusions

In the present study, axial tensile behavior of single walled silicon nanotubes is studied by implementing molecular dynamics simulations. The simulation is done using Lammmps software based on the Tersoff-Brenner many-body potential. The stress-strain behavior and subsequently the Young’s modulus of SiNTs are calculated by extracting the second derivative of the fitted polynomial curve to the strain energy. It is demonstrated that the developed results are in a very good agreement with available data in the literature. It is also found that the tube diameter has a small effect on the Young’s modulus.
References


