Computer Simulation of Buckling Behavior of SiC Nanotubes via Molecular Dynamics Theory

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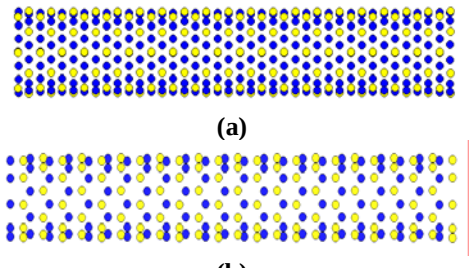
Abstract

In this paper the mechanical behavior of silicon carbide (SiC) nanotubes are investigated by molecular dynamics which an effective and accurate way of modeling the behavior of nanostructures. The interactions of atoms in SiCNT are described using the Tersoff potential. In this study both armchair and zigzag SiC nanotubes are considered. At first, the tensile behavior of single-walled SiCNTs is simulated. The generated results show that the Young's modulus of SiCNTs is in the range of 565 ± 50 GPa.
At the second stage, critical buckling load in axial compression for different length of armchair and zigzag SiCNTs are determined and the effects of nanotube length on the buckling behavior are studied. Simulations show that the critical buckling load decreases with the increase of nanotubes length. Also the results demonstrate that the critical buckling load in armchair (7,7) is lower than that of zigzag (12,0).

I. Introduction

SiC is considered to be promising material for high temperature, high frequency, and in harsh environment because of its out standing physical, chemical, and thermal properties [1]. Nanostructure of SiC such as nanotubes, nanowires and nanorods have been wide spread interest since the discovery of carbon nanotubes. These nanoscale materials show physical properties different from the bulk [2].
The structure of nanotubes was first constructed from graphitic SiC sheet. By analogy with CNT, single–wall SiC nanotubes are characterized by the pair of helical indices (*n*,*m*) which correspond to the circumference of the nanotube on to the sheet: (n,m=n) armchair, (n,m=0) zigzag. An example of SiC nanotubes is shown in Fig. 1.



(a)

(b)

Figure 1. The configuration of SiC nanotubes a) (7,7) SiCNT b) (12.0) SiCNT

Regarding the CNTs, many researches have been performed [3-5]. However, a few studies have dealt with the mechanical behavior of SiCNTs.
Miyamoto et al. [6] theoretically investigated the possibility of forming SiC nanotubes using density functional theory with the local density approximation. They demonstrated that the strain energy of SiC nanotubes is lower than of CNTs. The lower strain energy suggests the possibility of forming SiC nanotubes.
Moon et al. [7] calculated Young's modulus for SiC nanotubes by molecular dynamics simulation (MD). Bamieir et al. [8] studied the elastic and electronic properties of SiC nanotubes by ab initio method and determined strain energy and Young's modulus for different diameter of nanotubes.
In this article, we study the mechanical properties of SiC nanotubes using MD method based on tersoff potential. Based on this methodology the Young's modulus for different structure, of SiC nanotubes is obtained. The numeric results compare with the results of other studies. Atomistic simulations are also performed to investigate the buckling behavior of

different type of SiC nanotubes (armchair, zigzag) under uniaxial compression.

II. SIMULATION DETAILS

Molecular dynamics is widely used in many numerical simulations of physical process. The simulation process can be divided into four sections; determination of the initial locations and velocities of atoms, the evolution of equilibrium state, the procedures for adding new external forces or external displacements, calculation and analysis.

The selection of potential function is a key factor which determinate the results accuracy in MD simulation. In this study, interactions between atoms are modeled with the classical multi body Tersoff potential [9], which can reliably describe the main features of the mechanical response of SiCNTs. The total potential energy E of the atomic bonds of a SiCNT is expressed as,

$$\sum_i E_i = \frac{1}{2}\sum_{i \neq j} V_{ij} \tag{1}$$

$$V_{ij} = f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \tag{2}$$

With

$$f_R(r_{ij}) = A_{ij}\exp(-\lambda_{ij} r_{ij})$$

$$f_A(r_{ij}) = B_{ij}\exp(-\mu_{ij} r_{ij})$$

$$f_c(r_{ij}) = \begin{cases} 1, r_{ij} < R_{ij} \\ \frac{1}{2} + \frac{1}{2}\cos[\pi(r_{ij} - R_{ij})/(S_{ij} - R_{ij})], R_{ij} < r_{ij} < S_{ij} \\ 0, r_{ij} > S_{ij} \end{cases}$$

Where V_{ij} is the bond energy, $f_c(r_{ij})$ is a truncation function and b_{ij} is the multi-body order parameter describing how the bond-formation energy is affected by the local atomic arrangement due to the presence of other neighboring atoms (the k-atoms). It is a multi-body function of the positions of the atoms i, j, and k, which has the form of,

$$b_{ij} = \chi_{ij}(1 + \beta_i^{n_i}\xi_{ij}^{n_i})^{-1/2n_i}, \tag{3}$$

$$\xi_{ij} = \sum_{k \neq i.j} f_C(r_{ij}) g(\theta_{ijk}), \tag{4}$$

$$g(\theta_{ijk}) = 1 + c_i^2/d_i^2 - c_i^2/[d_i^2 + (h_i - \cos\theta_{ijk})^2] \tag{5}$$

$$\lambda_{ij} = (\lambda_i + \lambda_j)/2, \tag{6}$$

$$\mu_{ij} = (\mu_i + \mu_j)/2, \tag{7}$$

$$A_{ij} = (A_i A_j)^{1/2}, B_{ij} = (B_i B_j)^{1/2} \tag{8}$$

$$R_{ij} = (R_i R_j)^{1/2}, S_{ij} = (S_i S_j)^{1/2} \tag{9}$$

Where, r_{ij} is the distance of the ith and jth atom, θ_{ijk} is the angle between r_{ij} and r_{ij}, $A_i, B_i, \mu_i, \lambda_i$, $\omega_{ij}, \chi_{ij}, \beta_i, n_i, c_i, d_i, h_i, R_{ij}$ and S_{ij} are some correlative constants with the C-Si system, and their values take the corresponding ones in Refs.[9-11].

Two sets of MD simulations are carried out as follows; (1) The armchair and zigzag SiCNTs of the same length with different diameters varying from 0.62nm to 1.63nm, respectively. (2) Considering (7,7) and (12,0) SiCNTs which means that nanotubes have identical diameter with length of varying from 6nm to 16nm. In the developed method, the atoms in the top end of these nanotubes are shifted downwards along the axis by 0.001nm in each step, and the whole tube is relaxed while keeping the two ends constrained. Each relaxation time is 0.8×10^{-3} ps and for solving the kinetic equation the Gear's algorithm is adopted.

III. RESULT AND DISCUSSION

At first, the mechanical properties of SiC nanotubes are investigated. Among these properties, young's modulus is one of the important characterizations of mechanical properties of materials. In classical mechanics the Young's modulus is defined as [12]

$$Y = \frac{\sigma}{\varepsilon} = \frac{F/A}{\Delta L/L_0} \tag{10}$$

where σ is the axial stress, ε is the strain, F is the axial tensile force acted on the object, A is the cross-sectional area of object, L_0 is the initial length and ΔL is the elongation under the force F. Based on this method, the Young's modulus of SiCNTs are studied. In this model, the cross-sectional area A is $2\pi R\delta R$, where R stands for the tube radius and δR stands for the wall thickness with a value of 0.34nm [9]. The stress–strain curve of armchair (7,7) SiCNTs is obtained and given in Fig. 2.

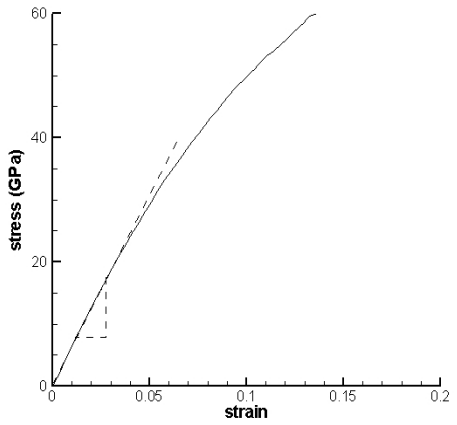


Figure 2. The stress-strain curve for SiCNT-Armchair (7,7)

It is seen in the Fig.2 that the elastic limit is at the strain value of 0.06. Beyond the elastic limit, the stress-strain curve deviate from a straight line. Computational results of Young's modulus of SiCNTs for different tube diameters are shown in Fig.3. There is a slight difference between the trends of variation in Young's modulus of armchair and zigzag SiCNTs. The Young's modulus of carbon nanotube is shown for comparison. Note that for the given diameter the Young's modulus of the SiC nanotubes is lower than that of the Carbon nanotubes. It is clear that, the numeric results for SiCNTs are in good agreement with the results of moon et al. [7].

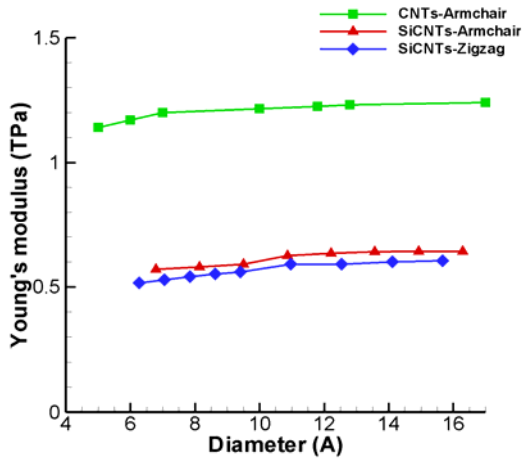


Figure 3. Young's modulus as a function of nanotube diameter. The value of carbon nanotubes is adapted from reference [13]

At the next stage, buckling of an armchair and zigzag nanotube under axial compression is investigated. The deformation configurations for the (7,7) tube are plotted in Fig. 4, which are very similar to carbon nanotubes that described by Xin et al. [14].

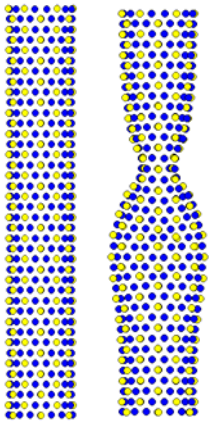


Figure 4.Typical configuration of SiCNT (7,7) a)Initial shape b)Buckling shape

Also, the load–strain curve for (12,0) SiCNT is obtained Fig.5. It is noticed that the axial load of the SiCNT increases linearly before the tube is compressed to the critical buckling strain.

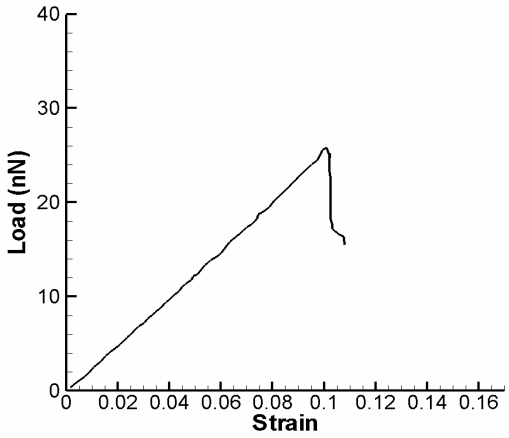


Figure 5. Buckling load-strain curve of SiCNT (12,0) with length 11.7 nm

Furthermore, MD simulations of axial compression are carried out on (7, 7) and (12, 0) SiCNTs with various lengths. The diameters of both (7, 7) and (12, 0)

SWCNTs are about 0.95 nm. In Fig.6 the critical buckling load of armchair and zigzag SiCNTs for lengths varying from 8nm to 16nm are obtained. In this figure the critical buckling load for carbon nanotubes are shown for comparison. According to the results, the SiC nanotubes show the same load trend in compared with Carbon nanotubes with various lengths [14]. The results exhibit that critical buckling load of SiCNTs are dependent on the length and chirality to a certain extent. Also, the critical buckling load decreases with the increase of nanotubes length and critical buckling load of zigzag SiCNT (12,0) is greater than that of armchair SiCNT (7,0).

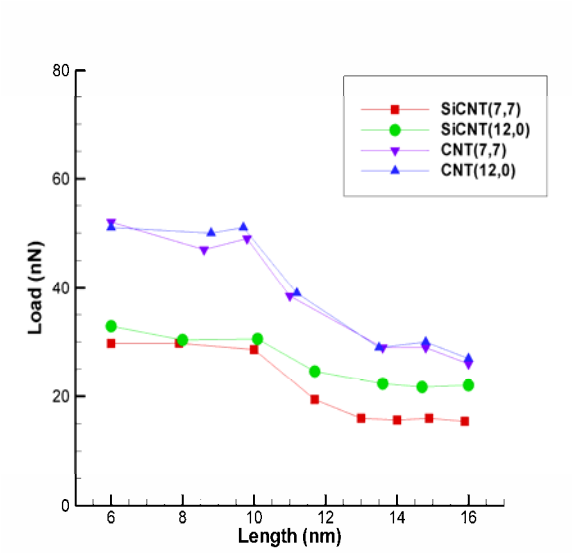


Figure 6. The variation of critical buckling load to the length for different SiCNTs and CNTs type

IV. CONCLUSION

The mechanical properties of SiC nanotubes were investigated using molecular dynamics simulation based on the Tersoff potential. In this regard, the Young's modulus of SiC nanotubes was estimated for different diameters. The simulations showed that the modulus of elasticity is weakly affected by the tube diameter. It was also found that the Young's modulus of SiCNTs is smaller than that of carbon nanotube.
Furthermore buckling behavior of (7,7) and (12,0) SiCNTs for different lengths under uniaxial compression were studied. The load-strain curve and the deformation shapes of (7,7) SiCNT were simulated. It was found that the critical buckling load of both (7,7) and (12,0) SiCNTs are related to the tube length. The generated results exhibited that the critical buckling load decreases with the increase of nanotube length. Also it was seen that the critical buckling load of SiCNTs was affected by the tube chirality.

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