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Critical Buckling Load of SiCNTs: A Molecular Dynamics Study on Gas Sensing

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Abstract

Silicon carbide nanotube (SiCNT) come forward in the great variety of nanotubes with higher durability until 1600 ^{o}C (in air) while carbon nanotube can stay stable until 600 ^{o}C (in air). First five buckling loads of single SiCNT placed between source and drain metal electrodes in nano sized field effect transistors (FET) is investigated using two different molecular dynamics methods. L.A.M.M.P.S. software and Gromacs package is used to perform molecular dynamics analyzes. Armchair structure of SiCNT with chiralities (10,0), (12, 0), (14, 0), (16, 0) were selected with 400, 480, 560, 640 atoms respectively. Results demonstrate clearly that longest nanotube perform lower stability as nanotubes becomes fragile with more atom numbers. Except from (10, 0) armchair SiCNT, first mode occurs at lowest load and rise as the number of mode arise.

Keywords: SiCNT, Field Effect Transistors, LAMMPS, Gromacs, MD Simulation.

1. Introduction

Fullerenes may be the first steps into nanomaterials which was emerged in the mid- 1980s. Krästschmer et al. [1] introduced the bulk production of fullerenes. Fullerene can be stated as an allotrope of carbon which consists of carbon atoms connected by both single and double bonds in shape of hollow sphere, ellipsoid, tube, or many other shapes. The interest in carbon nanomaterials remained limited as the potential were not fully understand. In 1991, with the discovery of carbon nanotube (CNT) by Iijima [2], carbon nanostructures gained wide interest all around the world due to superior mechanical properties. In 2008, Wu et al. [3] presented the potential of using silicon carbide nanotube (SiCNT) in gas sensors. It is presented that CO and HCN molecules can be absorbed to Si atoms on the wall of SiCNTs with binding energies as high as 0.70 eV and can attract finite charge from SiCNTs. The potential of sensitivity and accurate results in gas sensing using SiCNT pointed researchers to further researches. In 2011, Wang and Liew [4] presented the SiCNT performing as a highly sensitive gas chemical sensor for formaldehyde comparing to CNT. The interaction between HCOH and SiCNTs was presented using density functional theory (DFT). Apart from absorbing CO and HCN molecules on SiCNT Jia et al. [5, 6] investigated the SO_2 absorbing potential on (5, 5) zigzag SiCNT using DFT. Chemisorbing of SO_2 molecules to the Si–C bonds of SiCNTs with a result of generating different charge distribution, resulting in the breaking of some S–C bonds. Recently, Lin et al. [7] presented that phosphorus-doped SiCNT (P-SiCNT) perform better than classical SiCNT on sensing SO_2 molecules using DFT and MD simulation methods. In 2022, Singh [8] investigated sulfur-doped SiCNT for detecting liquefied petroleum gas at room temperature.

Composites of silicon based nanostructures with carbon based structures gained attention. Dzunda et al. [9] investigated the mechanical, physical properties and tribological behavior of four types of silicon carbide composites with addition of carbon nanotubes to enhance the electrical conductivity of nanotube. For two composites electrical conductivity reached values of 1448 S/m and 2873 S/m. Shen et al. [10] investigated the fatigue strengthening of carbon/carbon composites modified with carbon nanotubes and silicon carbide nanowires. Taguchi et al. [11] presented the synthesis of a novel hybrid carbon nanomaterials inside silicon carbide nanotubes using ion irradiation of a C-SiC coaxial nanotube with 200-keV Si ions at room temperature. Taguchi et al. accomplished to obtain one-dimensionally stacked graphene nanodisks with diameters less than 50 nm with cylindrical MWCNTs, inside an amorphous SiCNT. Tony et al. [12], using microwave heating, presented the synthesis of one-dimensional silicon carbide nanomaterial from the blend of SiO_2 particles with two types of CNTs. This work demonstrated that types of one dimensional SiCNWs (hollow or solid) can be selected using various types of CNTs together with proposing a high efficiency microwave heating method. Uzun [13] presented the production of reinforced aluminum foam using SiC particles and CNT together and separately. Powder metallurgy method was used to produce SiC particles and CNT reinforced aluminum foam. It is clearly demonstrated that addition of reinforcing affected the elastic–plastic deformation behavior. Yang et al. [14] presented the electromagnetic-shielding of CNT/graphene foam (GF)/SiC composites by in-situ growth of CNT in GF resulting in superior electromagnetic interface (EMI) shielding effectiveness (SE). Zhang et al. [15] developed a one-step method to synthesize Si/CNTs nanocomposite. A magnesium reduction process was developed using SiO_2 particles. Si/SiC/CNT nanocomposite were obtained for using in lithium ion batteries (LIBs) with a stable capacity of ~1100 mAh g^{-1} together with a capacity retention of about 83.8% at a current density of 100 mA g^{-1} after 200 cycles.

As setting up a new laboratory to perform nano sized analyzes can reach astronomical costs, researchers prefer to perform analyzes using classical mechanic [16-19] which leads to give non-accurate results, higher order continuum mechanics theories such as strain gradient [20-23], couple stress [21, 24-26], nonlocal elasticity [27-30], surface elasticity [31-35] etc. Furthermore, finite element [36, 37] and DSC method [38-43] methods were also used to perform analyzes without the need of a lab. On the other hand, modal and bending analyzes of nanostructures has been one of the most applied investigation on nanostructures [44-52].Theoretical works were promising in case of the ability to perform hundreds of analyzes in very short time [38, 53-61]. The most important disadvantage in theoretical works were the accuracy of methods used. It is not always possible to check the accuracy of method for each samples analyzed.

Molecular dynamics (MD) methods differ from other methods as researchers have the ability to model each atom separately. This ability leads to very accurate result with a usage of valid model. The interaction between both bonded and non-bonded atom is modeled in MD simulations. Another advantage of modeling each atom separately is to model imperfect nanostructures such as damaged structures or particular nanostuctures.

2. Silicon Carbide Nanotube (SiCNT)

Carbon based nanostructures such as graphene, fullerene, and CNTs has been the keystone of nanomaterials. First, with Young's modulus around 1000 GPa, CNTs attracted attention for a limited variety of potential using area with very high surface to volume ratio. After years, extraordinary electrical conductivity of CNT were introduced. Together with superior mechanical properties, electrical conductivity improved the interest to nanostructures drastically. Superior conductivity with very high durability made possible to use nanostuctures

in microelectromechanical (MEMS) and nanoelectromechanical systems (NEMS). Furthermore, the resistance to high-temperature of CNT and carbon based nanomaterials were limited. Due to the limited durability in high temperatures, scientists have developed a new structure of nanotube [62-64]. The structure consist of silicon (Si) atoms together with carbon atoms. Si atoms bonded to C atoms formed a novel structure in sheet form called silicon carbide sheet. Analyzes demonstrated that the durability under very-high temperatures were promising while the mechanical strength were not as high as fully carbon based structures. Silicon carbide nanotubes (SiCNTs) can be obtained by simply rolling silicon carbide sheets. SiCNT can keep stable until 1600 ºC (in air), whereas Carbon nanotubes were limited to stay stable until 600 ºC [65, 66]. Silicon based structures come forward with its strength to high temperature. In Fig. 1, the process of obtaining SiCNT from silicon carbide sheet is demonstrated. As it can be seen, the easiest way to obtain nanotube from nanosheet is to simply roll the flat structure until bonding.

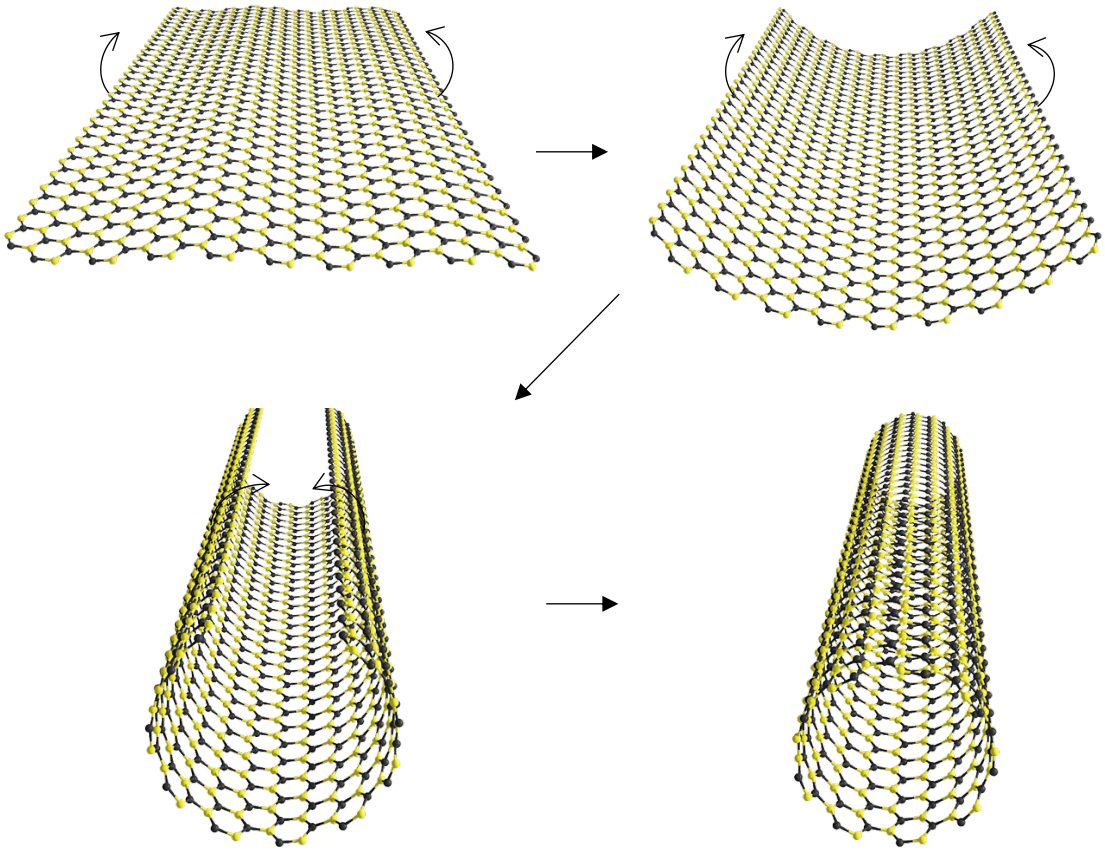


Fig. 1. Producing SiCNT from Silicon Carbide Sheet

Modeling nanotubes using continuum mechanic and MD simulation has great difference. As it can be clearly seen from bottom part of Fig. 2, the nanotube transform to cylindrical homogenous structure in continuum mechanic. This can lead to non-accurate results. On the other side, as it can be seen from the top part of Fig. 2, modeling each atoms separately in MD simulation would lead to more accurate results.

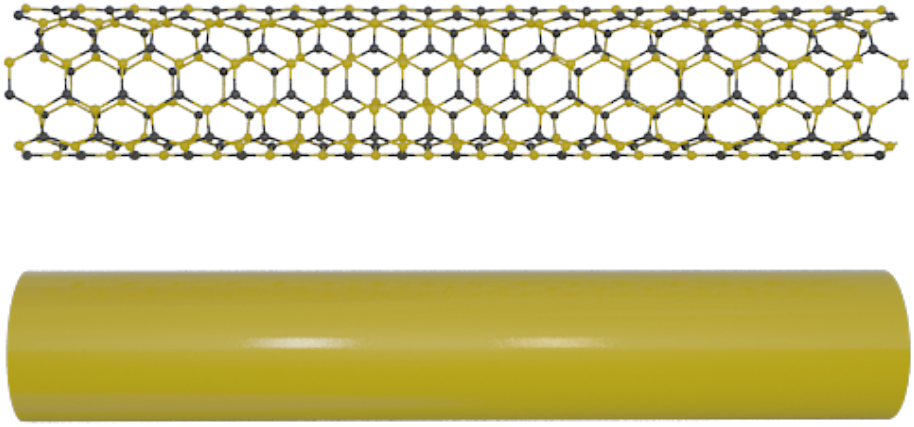


Fig. 2. Modeling SiCNT on MD simulation (top) and continuum mechanic (bottom)

Nanostructures can be presented using three main groups comparing bonding angles. The angle of nanostructures are rolled is represented by a pair of indices *(n,m)*. Here *'n and m'* denote the number of unit vectors along two directions in the hexagonal structures of silicon carbide sheet. As it can be seen in Fig. 3, if *m=0,* the structure is called *zigzag*, and if *n=m*, the structure is called *armchair*. In any other case, the structure will be called *chiral*. Armchair, zigzag, and chiral nanotubes have different physical, mechanical, and electrical properties which are neglected in continuum mechanic. In analyzes, SiCNTs with (10, 0), (12, 0), (14, 0), (16, 0) chirality of nanotubes are examined with following given stoichiometries in Table 1.

Table 1. Stoichiometries of SiCNTs

Chirality	Diameter (nm)	Numbers of atoms in sample
(10, 0)	0.9924	400
(12, 0)	1.1091	480
(14, 0)	1.3893	560
(16, 0)	1.5878	640

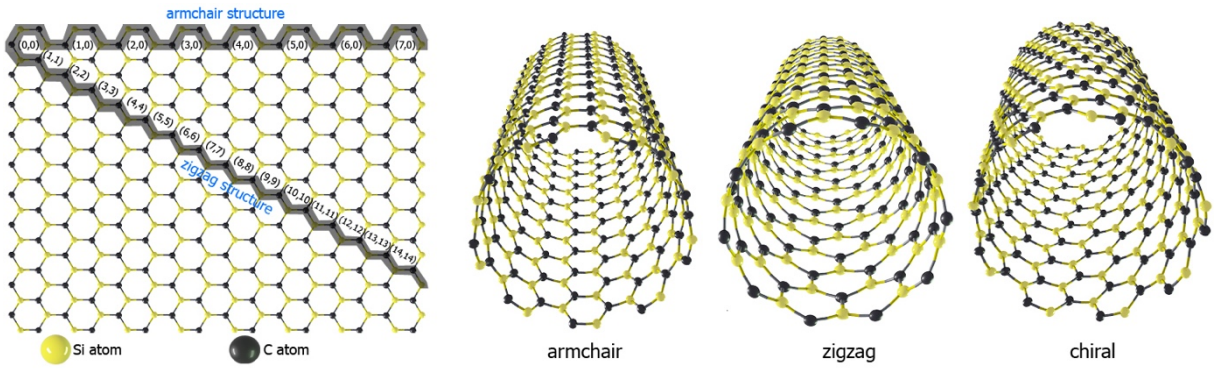


Fig. 3. Armchair, zigzag, and chiral SiCNT [65]

Silicon carbide nanostructures are widely used in gas sensors due to its durability under high temperature [67]. CO and HCN gases can be captivated on SiCNT at Si lattice sites in sensors. Any captivation on sensor leads to fluctuation in binding energy. Fluctuation in binding energy change the conductivity of SiCNT on sensor. Electro-transducers measures the absorbed gas molecules [68]. Field effect transistors (FET) is presented in Fig. 4. As it can be seen from Fig. 4 the nanotube take place between source and drain metal electrodes.

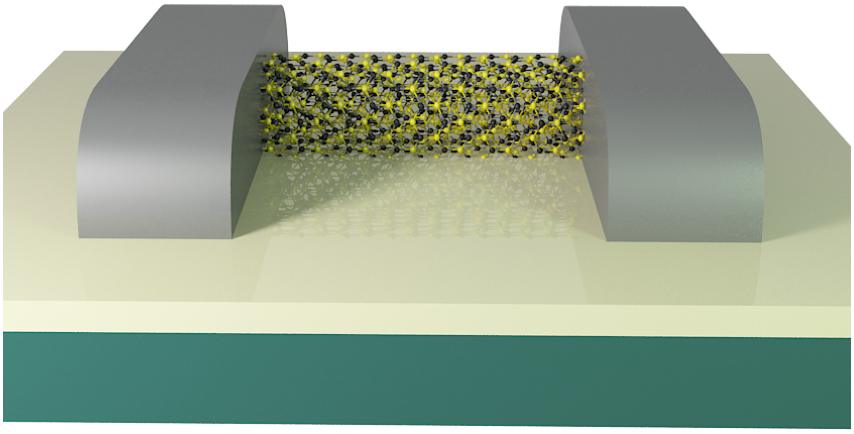


Fig. 4. SiCNT in NEMS

3. Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

Molecular dynamics (MD) method allows to examine the material properties and dynamic behavior of nanoscaled structures such as nanotubes, nanoplates etc. MD differ from other methods in case of the ability to calculate each samples material properties separately from the interactions between atoms. This create the opportunity to be able to analyze imperfect structures with more accurate results. The reactive empirical bond order potential (REBO) which was exposed by Brenner in 1990 can be accepted as the starting point of calculating potential between atoms of hydrocarbons including nonlocal effect [69]. REBO is based on Tersoff's covalent-bonding formalism and include extra terms for correcting overbinding. In our previous work, interatomical potentials calculations was expressed as follow [70]:

$$2E = \sum_i \quad \sum_{j\neq 1} f_c(r_{ij}) \quad \left(f_T(r_{ij}) + b_{ij} f_E(r_{ij})\right) \tag{1}$$

Where

$$f_T(r\ ) = Ae^{(-\lambda_1 r)} \tag{2}$$

$$f_E(r\ ) = -Be^{(-\lambda_2 r)} \tag{3}$$

$$f_C(r\ ) = \begin{cases} 1 & : r < R - D \\ 0.5 - 0.5sin\left(\frac{\pi}{2}\left(\frac{r-D}{D}\right)\right) & : R - D < r < R + D \\ 0 & : r > R + D \end{cases} \quad (4)$$

$$b_{ij} = \sqrt[2n]{\frac{1}{1+\beta^n \xi_{ij}^n}} \quad (5)$$

$$\xi_{ij} = \sum_{k\neq i,j} f_C(r_{ij}) g(\theta_{ijk})\, e^{\lambda_3^m (r_{ij}-r_{ik})^m} \quad (6)$$

$$g(\theta) = \gamma_{ijk}\left(1 + \frac{c^2}{d^2} - \frac{c^2}{d^2+(cos\theta - cos\theta_0)^2}\right) \quad (7)$$

Where i,j and k represent the atom numbers, θ is the angle between atoms, r is the distance between Si and C atoms. Furthermore, f_T act in place of a two-body term, f_C represent cutoff term while f_E stand for three-body interactions.

4. Gromacs Package

Gromacs is a package which allow to perform molecular dynamics analyzes using interactions between neighboring atoms. Nanotubes were modeled subjected to compressive loading with different geometric parameters. To calculate the interactions between atoms, the force potentials from both bonding together with nonbonding interactions needs to be taken into consideration. Non-bonding interactions occurs due to van der Waals force instead of electrostatic interactions. Assorted potential functions can be used to obtain forces needed. In this paper Lennard-Jones potentials were used. The equation of motion to obtain the i^{th} atoms force can be stated as

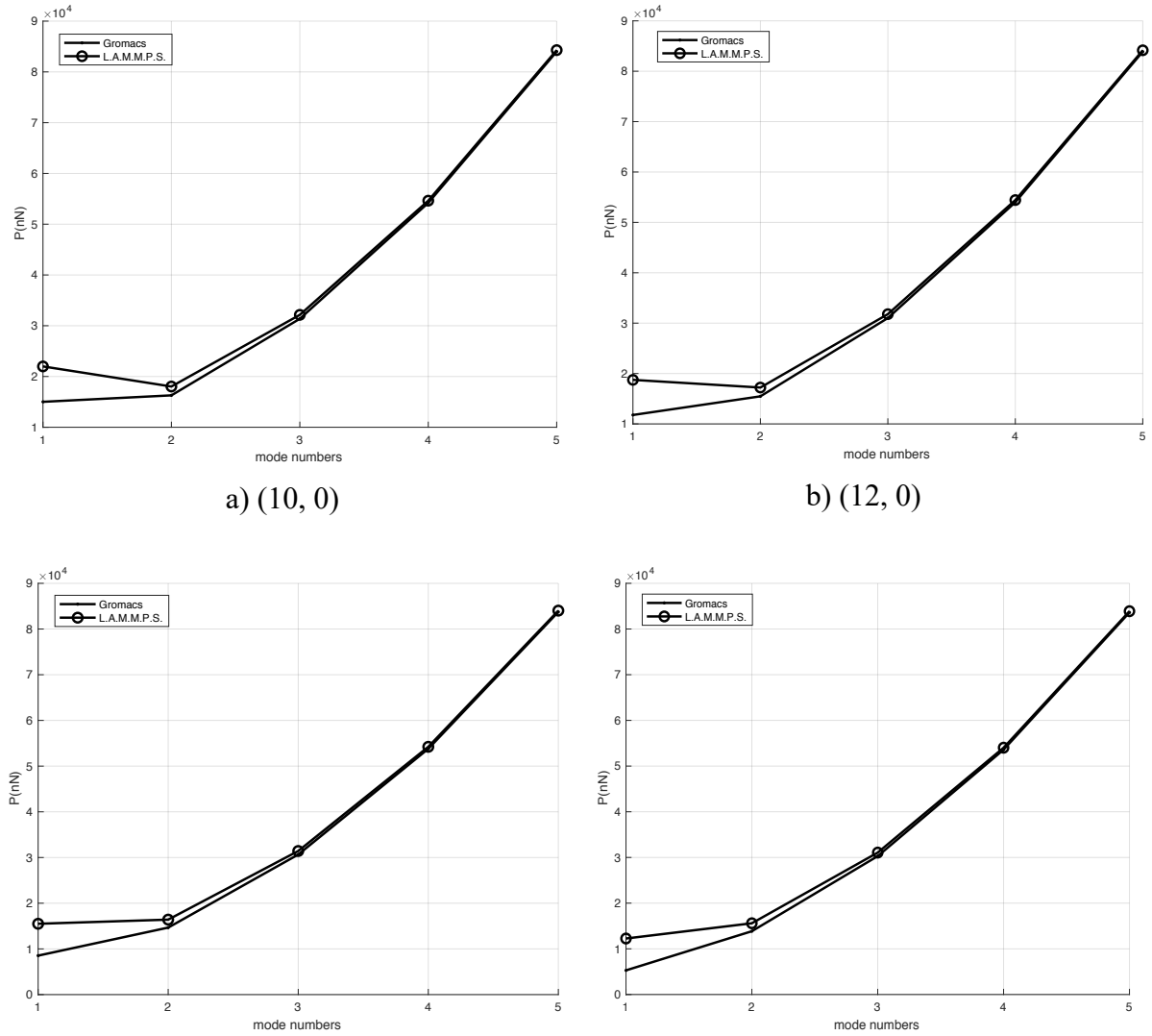
$$F_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{\partial \emptyset_{ij}(r_{ij})}{\partial r_{ij}} \frac{r_j - (r_i)}{|r_j - (r_i)|} \quad (8)$$

Whilst dynamical process, the location of calculated i^{th} atom were presented as $r_i(t)$ at specific time (t). Newton's second law were followed on the differ in atomic positions leading to capturing the fluctuation in the energy of the system. Small time steps were applied to capture the fluctuation as follows together with Verlet algorithm to reduce computational time

$$F_i = m_i \frac{\partial^2 r_i}{\partial t^2}, \quad i = 1,2,\ldots,N \quad (9)$$

4. Numerical Results

In this section the comparative buckling analysis of SiCNT using L.A.M.M.P.S and Gromacs package is presented. Armchair SiCNT structures with chiralities (10, 0), (12, 0), (14, 0), (16, 0) are examined. Calculated Young's modulus of SiCNTs with (10, 0), (12, 0), (14, 0), (16, 0) chirality varies from 508.3 GPa to 518.1 GPa.



a) (10, 0) b) (12, 0)

c) (14, 0) d) (16, 0)

Fig. 5. First five modes of stability analysis

Armchair (16, 0) SiCNT with 640 atoms perform lowest stability comparing to other structures for both MD simulation results while (10, 0) with 400 atoms perform highest stability. L.A.M.M.P.S. analysis for (10, 0) armchair SiCNT results in lower second mode which means second mode shape occurs before first mode of buckling while Gromacs differ from L.A.M.M.P.S. in this analysis. Results are plotted for first five modes of (10,0), (12, 0), (14, 0), (16, 0) in Fig. 5 (a-d) respectively.

5. Conclusions

As biocompatible materials, SiC nanostructures have many applications in biomedicine. SiC is used in coatings on biomedical implants with excellent wear-resistant and non-hazardous to health, also SiC films with very small pores are used as semi-permeable biomaterials. Biomorphic SiC ceramics coated with bioactive glass show great promise as dental and orthopedic implants with improved mechanical and chemical properties. In current work

SiCNTs stability analysis is investigated using two different molecular dynamics packages. Results indicates that the size of nanotube effect the stability as nanotubes becomes fragile with more atom numbers. Except from (10, 0) armchair SiCNT, first mode occurs at lowest load and rise as the number of mode arise.

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