Examining Mechanical Properties of Silicon Nano-tubes by Molecular Dynamic Theory

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Abstract: The mechanical behavior of silicon nanotubesis studied using molecular dynamics based on the tersoff potential. The variation of Young's modulus versus temperature and diameter is obtained. The results show the diameter variation does not affect the Young's modulus significantly. Then, the buckling behavior of Si nano-tube under uniaxial loading is simulated, and the critical buckling load and strain are computed. The effects of length, diameter and strain rate on critical buckling load and strain are studied. In addition, the effect of defect on buckling behavior is investigated.

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1. Introduction

Since the invention of carbon nano-tubes in 1990, different theoretical and experimental methods have been used to analyze and model them. Carbon nano-tubes are theoretically produced by tubing graphitic planes. They are used to manufacture nanocomposites, nanosensors and microscopic props [1]. Currently, nanotubes are made of silicon carbide (SiC) and silicon germanium (SiGe) in addition to carbon nanotubes and their mechanical behavior has been studied [3,2].

Single-dimension Silicon nanomaterials, such as nanotubes and nanowires, have particular mechanical, thermal, optical and electric properties and potential applications in the industry [4]. Using the theory of quantum mechanics, Fagan et al [5] showed stability and manufacturability of silicon nanotubes. Sha et al [6] produced silicon nanotubes by chemical vapor analysis using a sublayer Al_2O_3. Chen et al [7] could manufacture silicon nanotubes by hydrothermal methods. Castrucci et al [8] confirmed silicon nanotubes by electron microscopes. Kang et al [9] calculated value of strain energy and Young's module for silicon nanotubes. Calculations showed that changes in diameter of silicon nanotubes did not considerably influence on strain energy of nanotubes. Zhang et al [10] compared stability of armchair and zigzag silicon nanotubes using density function. Findings show that armchair silicon nanotubes are more stable than zigzag ones.

Seifert et al [11] examined electronic and mechanic properties of charged and hydrogenised silicon nanotubes. Li et al [12] evaluated geometry of silicon nanotubes containing silicon rings. Findings show that ringed silicon nanotubes are structurally stable. Jeng et al [13] studied the effects of strain rate and network failure on tensile behavior of silicon nanotubes by molecular dynamic theory. Findings showed that increase in strain rate of nanotubes increased their tensile resistance; while network failure resulted in decline of tensile resistance.

The present study examines mechanical behavior of armchair silicon nanotubes by molecular dynamic theory. The theory calculates elasticity factor of silicon nanotubes per different diameters and temperatures. The current study examined the effect of parameters including length and strain rate on buckling behavior of silicon nanotubes and calculated the effect of diameter on buckling critical strain of silicon nanotubes. The study also obtained values of buckling critical load for failed silicon nanotubes per different failures.

2. Problem Solution

Molecular dynamic theory is a proper method to model material behavior in Nano sizes. This method studies movement of an atom using classic mechanics and Newton's movement equations. Molecular dynamic theory has been used to predict mechanical and physical properties of most nanostructures including nano-tubes and nanowires [14].

The present study used molecular dynamic method based on Tersoff potential function to simulate silicon nano-tubes. In this function, potential of inter-atomic forces depends on location and bond angle of silicon atoms. In the Tersoff potential function, bond energy related to i^{th} and j^{th} silicon atom is calculated by Equation 1:

$$V_{ij} = f_C(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})] \quad (1)$$

According to above, V_{ij} is bond energy of atoms, r_{ij} is the distance between atoms, f_R is the function indicating inter-atomic repulsive energy, the function f_A indicates inter-atomic attractive force and the f_C is the shear function. The factor b_{ij} is a function of bond angles of atoms indicating that bond forces depend on bond angle of atoms by their neighbors. The factor b_{ij} is as follows:

$$b_{ij} = (1 + \beta^n \xi_{ij}^n)^{-1/2n} \quad (2)$$

where:

$$\xi_{ij} = \sum_{k \neq i,j} f_c(r_{ik}) g(\theta_{ijk}) \exp\left[\lambda^3 (r_{ij} - r_{ik})^3\right] \quad (3)$$

$$g(\theta) = 1 + c^2/d^2 - c^2/[d^2 + (h - cos\theta)^2] \quad (4)$$

where θ_{ijk} is the angle between the bonds ik, ij and the factors d, c, λ, n, β are constants related to atomic bond [15].

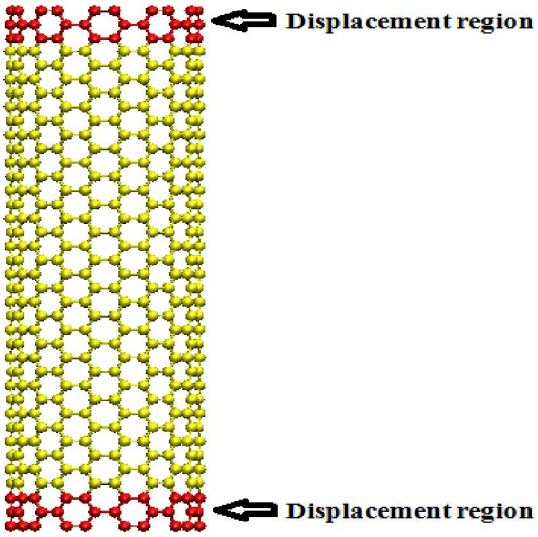

Figure 1: Primary structure of silicon nano-tubes influenced by boundary conditions

Through simulation, silicon nano-tubes are balanced in a certain temperature for 10^6 time step. Balancing results in elimination of primary tensions. As the system balances, boundary conditions are imposed on two tips of silicon nano-tubes in the form of displacement. After displacements, balancing occurs for 0.5 μs again followed by displacement. System temperature is controlled by scale thermostat. This thermostat which is the simplest one scales velocity of a particle per time step so that system temperature remains constant. The equation is as follows:

$$v_i^{new} = v_i^{old} \sqrt{\frac{T_0}{T}} \quad (5)$$

where T_0 is system temperature, v_i^{old} and v_i^{new} are velocity of i^{th} particle pre and post scaling, respectively. Figure 1 shows primary structure of silicon nano-tubes and areas which are influenced by boundary conditions.

3. Results

This section represents results from modeling armchair silicon nano-tubes. First, values of elasticity factor are calculated for different diameters and temperatures. Then, buckling behavior of armchair silicon nano-tubes is studied by molecular dynamic theory. Finally, the effect of different network failures is examined on buckling critical load.

3.1. Calculating Elasticity Factor of Armchair Silicon Nano-tubes

This section studies values of elasticity factor of silicon nano-tubes for different diameters and temperatures. Elasticity factor is obtained as follows:

$$E = \frac{\sigma}{\varepsilon} = \frac{F/A}{\Delta L/L_0} \quad (6)$$

where, σ is normal tension, ε is normal strain, F is axial force, A is cross-sectional area, ΔL is changes in length of nano-tubes and L_0 is the primary length of nano-tube. To calculate elasticity factor, tension is diagramed versus strain for silicon nano-tubes; then gradient is considered as the elasticity factor. According to above equation, to calculate tension needs cross-sectional area of silicon nano-tube which is obtained as follows:

$$A = \pi t D \quad (7)$$

where, t is wall thickness and D is the tube diameter. Wall thickness of silicon nano-tubes are considered approximately equal to that of graphitic planes [13].

Here, tensile behavior of 15 nm armchair silicon nano-tubes is modeled for different diameters in 0.01 and 300 K°. Boundary conditions is imposed that during each time step two tips of the nano-tube are 3.8×10^{-4} nm displaced. As system balanced, above displacement is again done on two tips.

Table 1 shows elasticity factor of silicon nano-tube (10,10) in 300 K° to validate modeling. The results are consistent with values reported in [13]. [13] examined tensile behavior of silicon nano-tubes; but

the present study examined their buckling behavior as well as their tensile properties.

Table 1: comparing obtained results with [13]

Silicon nano-tube (10,10)	Elasticity factor (GPa)	Diameter (nm)
Present model	52.9	2.1
[13]	59.36	2.205

Figure 2 shows tension diagram versus strain for silicon nano-tube (10,10) in 0.01 K°. As the diagram shows, tension first increases linearly versus strain; then, the tube is ruptured in the strain 0.133. Gradient of linear part is 82 GPa indicating elasticity factor of the nano-tube.

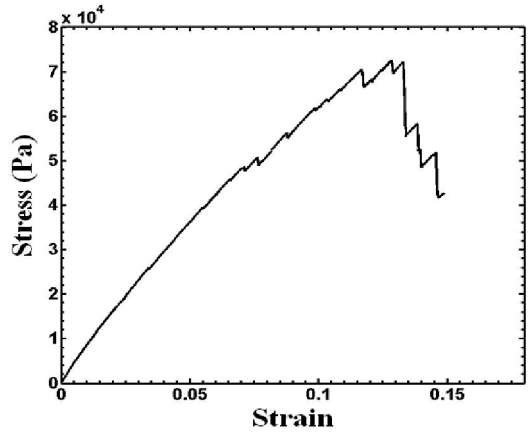

Figure 2: tension changes versus strain for silicon nano-tubes (10,10) under tensile load

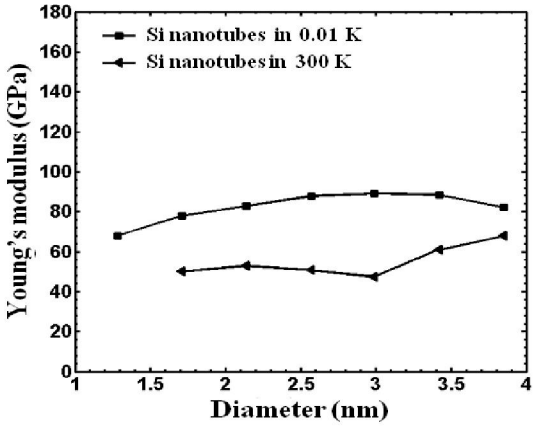

Figure 3: changes in elasticity factor of silicon nano-tubes versus diameter in 0.01 and 300 K°

Figure 3 shows elasticity factor of silicon nano-tubes for different diameters in 0.01 and 300 K°. The diagram shows that increase in system temperature causes decrease in elasticity factor of silicon nano-tubes. As a result, elasticity factor is approximately 82.2 and 54.4 GPa in 0.01 and 300 K°, respectively. Clearly, changes in diameter of armchair silicon nano-tubes do not considerably influence on elasticity factor.

3.2. Buckling of Armchair Silicon Nano-tubes in Different Lengths

Here, buckling behavior of silicon nano-tube (10,10) is studied for different sizes. Thus, one side of silicon nano-tube remains stationary and the other side is vertically displaced for 0.01 nm. As displacements are done, system is balanced for 0.5 μs.

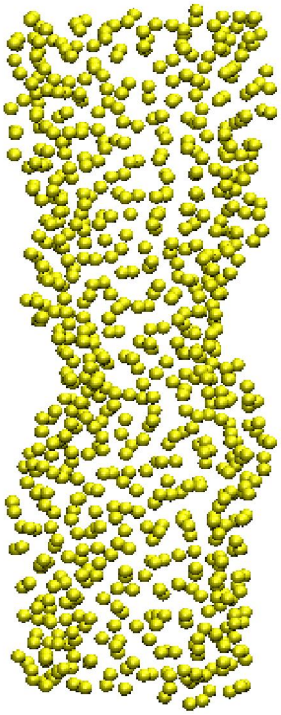

Figure 4: transformation of silicon nano-tubes as buckling occurs.

Figure 4 shows transformation of silicon nano-tubes as buckling is occurred under axial load. Figure 5 shows load changes versus strain for 7.2 and 8.8 nm silicon nano-tubes (10,10). For 7.2 nm silicon nano-tube, strain is increased to 0.056; then the diagram suddenly drops which indicates buckling started in nano-tube. Buckling critical load, in this situation, is 12.9 nano Newton. For 8.8 nm silicon nanotube, the diagram drops in the strain 0.057 and buckling critical load is 9.6 nano Newton.

Figure 6 indicates buckling critical loads of silicon nano-tubes (10,10) for the range of 60-111 A° in length. Clearly, as the length of silicon nano-tube increases, buckling critical load decreases; so that buckling critical load for 6 and 11 nm silicon nano-tube (10,10) is 12.2 and 6 nano Newton, respectively.

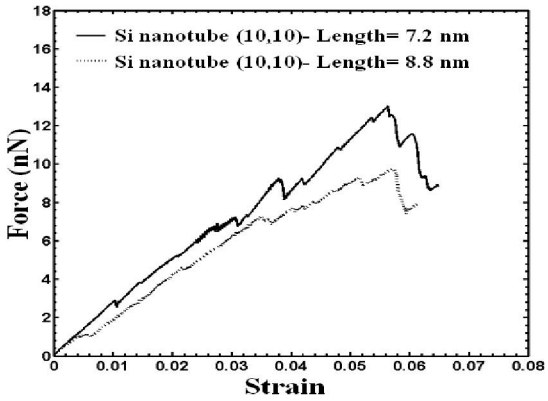

Figure 5: changes in the force versus strain for 7.2 and 8.8 nm silicon nano-tubes (10,10)

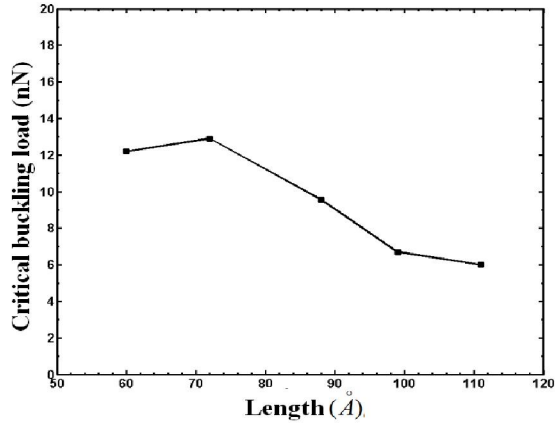

Figure 6: changes in buckling critical load versus length for silicon nano-tubes (10,10)

Figure 7 shows buckling critical strain versus length of silicon nano-tubes (10,10). Clearly, buckling critical strain does not considerably change in 60-88 A° and decreases for lengths > 88 A°. Changes in buckling critical strain and critical load is similar for silicon nano-tubes (10,10); thus, as the length increases, the two quantity decrease.

3.3. Buckling of Silicon Nano-tubes in Different Diameters

Here, buckling behavior of silicon nano-tubes is studied in 0.01 K° and for different diameters. To create axial load in the system, one side of the silicon nano-tube is unchanged and the other side is 0.01 nm displaced. The length of nano-tube here is considered as 7.2 nm. As the diameter of silicon nano-tube increases, its mechanical behavior approaches to that of flat silicon planes. Thus, it is expected that as diameter increases buckling critical load decreases. Figure 8 shows changes in buckling critical load of silicon nano-tubes versus diameter. The results show that as diameter increases buckling critical load decreases. Obviously, as diameter increases in the range of 2.14-3.85 nm buckling critical load decreases about 16%.

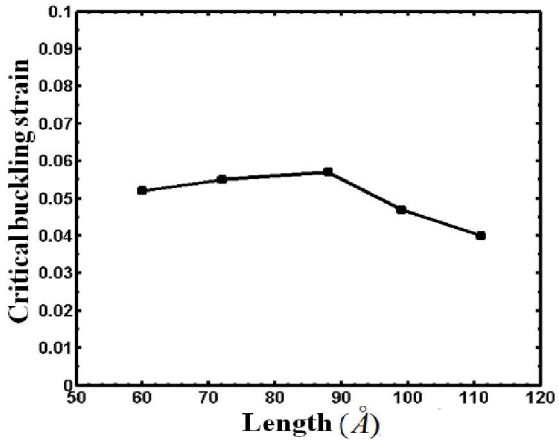

Figure 7: changes in buckling critical strain versus length for silicon nano-tubes (10,10)

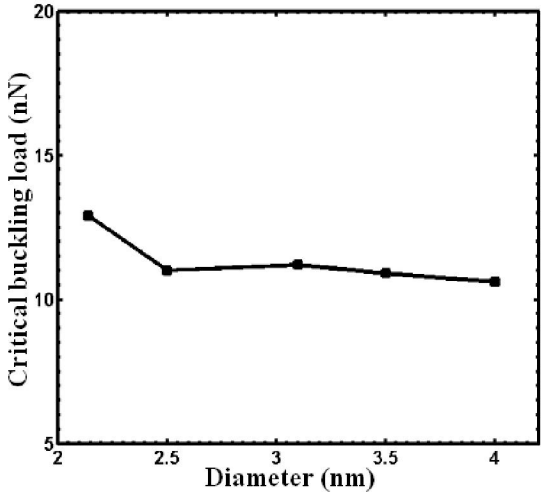

Figure 8: changes in buckling critical load versus diameter

Figure 9 shows buckling critical strains versus diameter. Obviously, as the diameter increases buckling critical strain decreases. Thus, for a 2.1 nm silicon nano-tube in diameter, buckling critical strain decreases approximately 0.055; while for 3.8 nm silicon nano-tube in diameter, this would decrease to 0.04.

3.4. The Effect of Strain Rate on Buckling Critical Load and Critical Strain

Here, buckling behavior of silicon nano-tubes (10,10) is studied in 0.01 K° versus different strains. The length of silicon nano-tube here is 7.2 nm and changes in strain rate are in the range of 1.3×10^{-5} to 7.4×10^{-4}.

As strain rate increases, there is no enough time to uniformly distribute tension in the whole structure

of nano-tube. This results in centered tension in the nano-tube. Figure 10 and 11 show changes in buckling critical load and critical strain versus strain rate. Obviously, changes in strain rate do not considerably influence on buckling critical load and critical strain. Average of buckling critical load and strain is 12.7 and 0.059 nano Newton, respectively in the range of 1.3×10^{-5} to 7.4×10^{-4} strain rate/s.

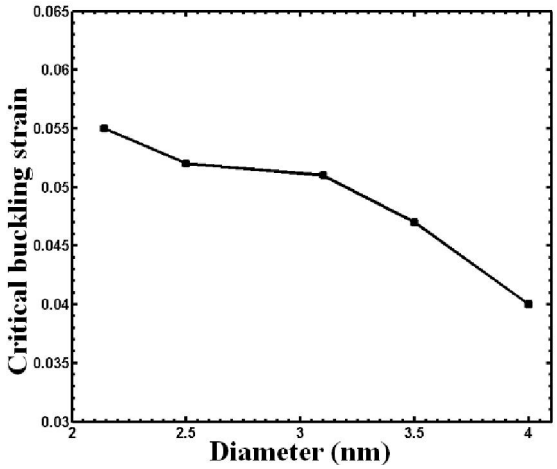

Figure 9: changes in buckling critical strain versus diameter

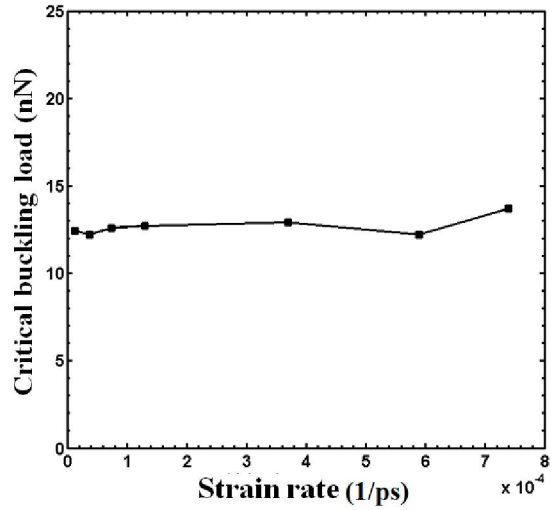

Figure 10: changes in buckling critical load versus strain rate for silicon nano-tubes (10,10)

3.5. Buckling Behavior of Silicon Nano-tubes with Failed Atomic Network

Naturally, failures happen in the atomic network of nano-tubes during production [16]. Failure in the network influences on buckling behavior of nano-tubes and their mechanical properties. Here, the effect of network failure is studied on 7.2 nm silicon nano-tubes (10,10) in 0.01 K°. Ends of the tubes are 0.01 nm displaced.

Through this study, as [13], network failures happened in silicon nano-tubes. That is, 1-8 % of atoms have been accidentally removed from nano-tubes; then system is under axial loading.

Figure 12 shows changes in buckling critical load for different failures. Obviously, as failure percentage increases, buckling critical load decreases. Buckling critical load for silicon nano-tubes (10,10) with 1% failure is 9.4 nano Newton; while it is 5.9 nano Newton for 8% failure. This sever fall is due to loosed structure of nano-tube under removing atom from primary structure.

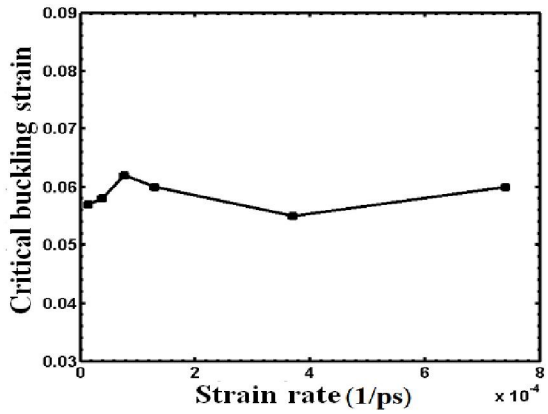

Figure 11: changes in buckling critical strain versus strain rate in silicon nano-tubes (10,10)

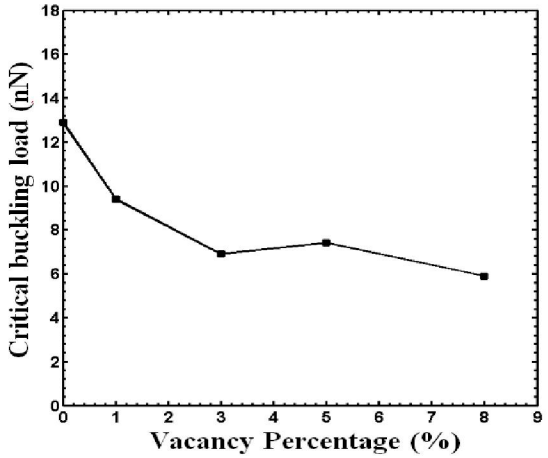

Figure 12: changes in buckling critical load for different network failure percentages

4. Conclusion

Present study examined mechanical behavior of armchair silicon nano-tubes under tensile and tension loads using molecular dynamic theory. It studied parameters including temperature, length, diameter and strain rate. Buckling behavior of silicon nano-tubes was examined for different atomic network failures. The results are as follows:

1. Diameter of armchair silicon nano-tubes does not considerably influence on elasticity factor.

2. Increase in system temperature does not severely decrease elasticity factor. That is, as system temperature increases from 0.01 to 300 K° elasticity factor decreases 34%, on average.

3. As length and diameter of silicon nano-tubes increase, buckling critical load and strain decrease.

4. Changes in strain rate do not considerably influence on buckling critical load and strain of armchair silicon nano-tubes.

5. Failure of armchair silicon nano-tubes severely decreases their buckling critical load; that is, 8% failure drops buckling critical load by 54%.

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