The Role of Stone-Wales Defects in the Mechanical Behavior of a Zigzag SWNT

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ABSTRACT

Using molecular dynamics simulation, we investigate the influence of Stone-Wales defects in the mechanical behavior of a zigzag (5,0) single walled carbon nanotube considering two different interatomic potential functions, the Tersoff-Brenner bond order potential and tight binding potential. The nanotube is subjected to axial stretch and the potential energy is computed for gradually increasing strain values. From the energy-strain curve the mechanical characteristics like Young's modulus, tensile strength and ductility are computed using both the potentials, firstly with a perfect lattice and then by introducing an increasing number of Stone-Wales defects. Significant reduction in the values of the mechanical properties is observed with changes in the plastic deformation pattern.

Keywords: Stone-Wales defects, Carbon nanotube, Mechanical properties

1 INTRODUCTION

Stone-Wales (SW) [1] defects that are either inherently present in the carbon nanotubes (CNTs) or introduced into them in the manufacturing process, degrade their mechanical properties to a large extent. Theoretical studies [2-7] show a wide range of Young's modulus from 0.1-5.5 TPa while tensile strength varies from 5-150 GPa. Theoretically overestimated values of nanotube properties can be attributed to the presence of various defects in the CNT structures. However, the bending and buckling of CNTs under large strains are shown in the experimental work of Falvo et al.[8]. Experimental evidences of topological defects in CNT samples were obtained by Ebbensen and Takada [9] in 1995 which was named as Stone-Wales [10] defect. and Miyamoto et al. [11]. The role of vacancy defects or holes on the mechanical properties of CNTs was studied in many theoretical investigations such as of Mielke et. al [12], Lee et. al. [13], Xiao and Hou [14] and Wang et. al [15]. In the Molecular Mechanics (MM) and Molecular Dynamics (MD) study of Belytschko et al. [16], effects of missing atom and SW defects on the failure pattern were studied. Their results were in good agreement with the experimental observations of Yu et al. [17] for Morse potential but not for Brenner potential. Mielke et. al [12] observed a 20-30% reduction of strain values by MM calculation and 14-27% reduction by Quantum Mechanical calculation for vacancy defects. Troya et. al.[18], Chandra et. al.[19] and Lu and Bhattacharya [20], observed in their calculations the effects of SW defects on the stiffness and maximum strain.

On the other hand Nardelli et. al. [21] observed SW transformations at small strain resulting necking phenomenon. The SW rotation at small strain value was also reported by Zhang et. al.[22] and Song et. al.[23]. Tserpes and Papanikos [24] used pair wise modified Morse potential to come to the conclusion that SW defects served as nucleation site for fracture. They also observed reduction in failure stress and strain for different types of nanotubes. Tight Binding MD simulation was carried out by Richard [25] to observe the decreasing effects of the SW defects on the failure strain value. Recently, using Tersoff-Brenner potential, Pozrikidis [26] has studied the effects of circumferential as well as inclined SW defects on the three kinds of SWNTs. As the exact knowledge of the stiffness or strength of the nanotubes is important for their use as the reinforcements in the next generation composites, and as the defects in general improve the adhesion of the CNTs to a polymer matrix [27] , the defects are deliberately introduced into CNTs to achieve certain functionality. Adding suitable number of SW

defects, a CNT can be fully exploited for various applications. In this paper the dependence of the mechanical properties on the SW defects of a zigzag single-walled carbon nanotube (SWCNT) is studied with Tersoff-Brenner (TB1) potential and Tight Binding potential (TB2) and the results are compared.

2 METHOD OF CALCULATION

We have used the potential form developed by Brenner [28] for hydrocarbon, known as Tersoff-Brenner potential and Tight- Binding [29] potential. Using the potentials, MD simulation is carried out on a (5,0) SWNT of length 21.3 Å and radius 1.96 Å (i.e. aspect ratio 10.87). We have taken 5 repeated units of the original building block of a (5,0) SWNT which contains 100 atoms. Keeping one end fixed, stress is applied on the other end of the tube. Berendsen thermostat is used to maintain 300 K. Stress was calculated from the energy value according to the relation $\sigma = 1/A\ (dE/d\varepsilon)$ where σ is the stress, A is the area of the annular cross-section of the tube and $(dE/d\varepsilon)$ is the slope of the energy-strain curve. ε represents the strain. Area of the annular cross-section of the tube is found as $A=2\pi r\delta r$ where r is the radius of the tube and δr, its wall thickness. We have taken δr as 0.066 nm, which is close to the radius of a free carbon atom as obtained by Yakobson, Brabec and Bernholc [2]. Young's modulus (Y) was found from the slope of the linear portion of the curve.

3 RESULTS AND DISCUSSION

Results of the MD simulations show a scattering of data in all respects. For 1and 2 defects, Young's modulus, failure stress and ductility show different values. The increase in energy for defective tubes shows that energy is required for the formation of Stone-Wales defects.

A pristine tube in our calculation has Young's modulus value of 1.44 TPa with bond order potential. It can sustain a strain upto 20% beyond which it breaks giving a maximum stress value of 144 GPa. In tight-binding calculation these values are 1.131 TPa, 18% and 161 GPa. In the second case (with TB2) the fall of stress-strain curve is sharper than that of the first case (with TB1). But both the fractures are brittle in nature [Fig.1,3]. The Young's modulus values are comparable to the experimentally obtained average value of 1.5 TPa for SWNTs by Krishnan et al. [30]. Our results are also in agreement with the experimental results of Wong [31], and Treacy[32]. Failure stress values can be compared with the experimental values of Demczyk [33] of 150±45 GPa. Quantum mechanical calculations [7, 18, 34] have also given the failure stress values more than 100 GPa. Though Yu et al. [17] got, maximum strain values in the range of 2-13% and failure stress from 11 to 63 GPa, Quantum mechanical calculations predicted the maximum strain in between 20% and 30% which are comparable to our results. In the above two cases, elastic behaviors are observed upto approximately 5% strain. For TB1, stress increases slowly upto 10% strain and then suddenly rises giving a peak value at 20%. For TB2 stress increases rapidly and then slowly after 10% strain. Here also a sudden rise is observed showing a peak at 18% strain.

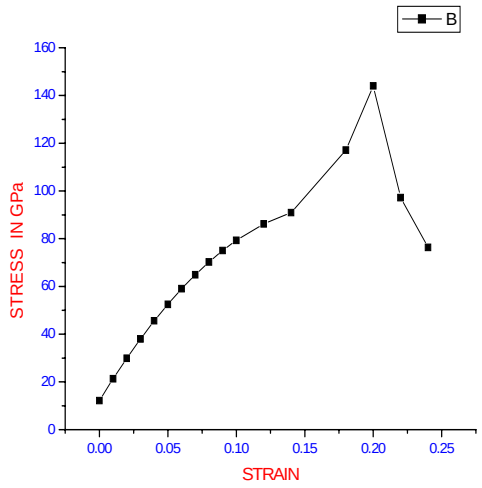

Fig.1: Stress-Strain curve of a (5,0) SWCNT without defect taking Bond Order potential

On straining the tube beyond 12% strain for a zigzag SWNT, as reported by Zhang et al. [22], SW rotation starts. After 20% (for TB1) and 18% (for TB2) strain values the tube breaks totally with the formation of a series of SW rotations.

When only one SW defect is introduced in the mid position of the CNT, the nature of the graph is changed markedly for TB2 but for TB1 the graph resembles with the graph of a perfect tube [Fig.2,4]. Ductility is reduced by 50% for TB2 showing the maximum strain value of 9%. The value is in the range of the experimental value of 2-13% by Yu et al. [17]. For TB1, this reduction is only 10%. Stiffness shows a reduction of 6% (TB1) and 23% (TB2). Failure stress in the first case is reduced from 144 GPa to 130 GPa and in the second case from 161 GPa to 106 GPa.. Here also, for TB2, the reduction is highest. Perfectly brittle rupture is observed with

TB1 for a defect free tube. Brittle, but not so sharp breaking mode is observed with TB1 by the introduction of 1 defect. For TB1, it can again be inferred that some SW rotations have occurred which results in the slow increase of the stress-strain curve in between 7% and 18%.

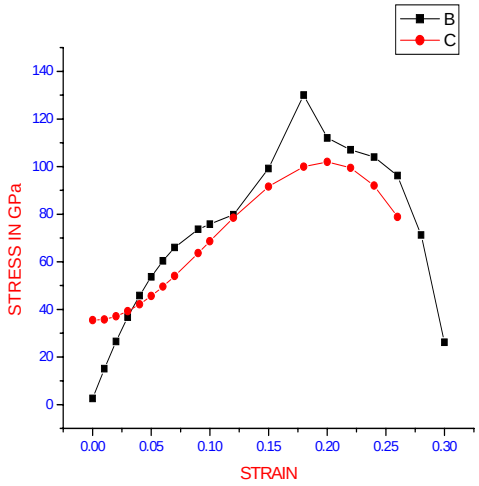

Fig: 2 Stress-Strain curve of a (5,0) SWCNT with defect (black-1 defect, red-2 defects)

To investigate the effects of even number of defects we have introduced two defects separated by some distance in the sample tube and get quite different stress-strain curves for TB1 and TB2 [Fig.2,4]. Maximum strain is 20% for TB1 and 19% for TB2. Failure stresses are 102 GPa and 103 GPa for the two cases respectively. Stiffness is also reduced by 14%. The result for 2 defects is clearly showing defect-defect correlation which comes into play for even number of defects.

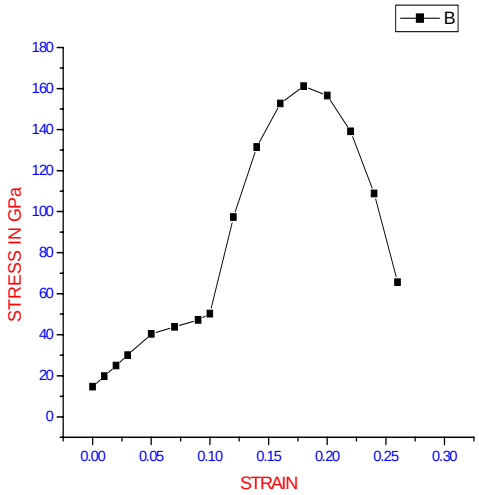

Fig 3: Stress-Strain curve of a (5,0) SWCNT without defect taking tight-binding potential

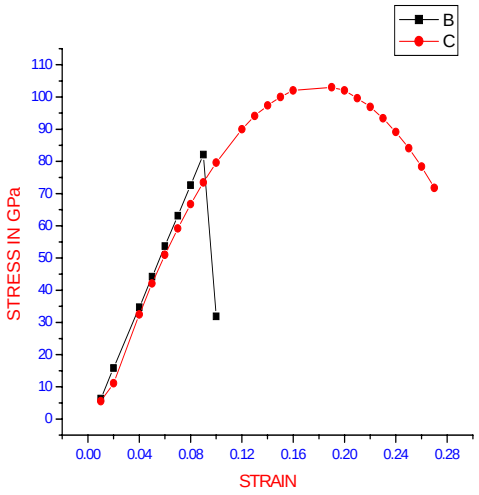

Fig 4: Stress-Strain curve of a (5,0) SWCNT with defect taking tight-binding potential (black-1 defect, red-2 defects)

According to Samsonidze Ge.G et. al [35], for a cylindrical geometry, double defect energy may be considered as a function of the distance between the defects and the tube radius. We have taken a small radius of the tube; hence the correlation between the defects has become significant. While straining the tube, this correlation is changed inside the tube complicatedly and ultimately results in improved ductility. Specially for TB2 the curve is changed dramatically by showing a increase in strain compared to the curve for 1 defect. While using TB1 we observed that the mode of fracture for a perfect SWCNT changes from a brittle fracture to a ductile one by the inclusion of SW defects. But the same change in pattern is not fully confirmed when we use TB2. With the presence of one SW defect the nanotube shows a sharp brittle fracture at a considerably small strain value, although when 2 SW defects are present the ductile nature is re-established. The results of our calculations are shown in Table 1 below.

4 CONCLUSIONS

Comparing the results of our calculations with two different interatomic potentials, it can be concluded that the inclusion of SW defects in a SWCNT structure, generally degrade their mechanical properties. Tight binding potential gives results which are closer to the experimental values regarding failure stress or ductility. So these calculations reveal that SW defects in one hand can serve as a main factor for the fracture of CNTs and on the other side, the introduction of suitable number of defects in proper positions may facilitate some specific applications.

	Bond Order Potential			Tight-Binding potential		
	Y value (TPa)	Failure Stress (GPa)	Maximum Strain	Y value (TPa)	Failure Stress (GPa)	Maximum Strain
Without defect	1.44	144	20%	1.131	161	18%
1 defect	1.35	130	18%	0.872	106	9%
2 defects	1.23	102	20%	0.851	103	19%

Table 1: Calculated mechanical characteristics of a SWCNT with and without SW defects.

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