Effect of Position and Orientation of Stone-Wales Defects on the Fracture Behavior of a Zigzag Single-Walled Carbon Nanotube

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ABSTRACT

Molecular dynamics simulation has been carried out to study the mechanical properties of a 42.59 Å long zigzag (10, 0) single-walled carbon nanotube with an increasing number of Stone-Wales defects, by varying their relative position and orientation. Brenner bond order potential has been employed for energy minimization. Changes in tensile failure stress, maximum strain and fracture behavior are reported in the present work. Maximum reduction of the tensile strength is observed for overlapping defects. Ductility of the tube is little affected by the presence of defect in the tube structure. Breaking patterns when modeled show variation in their initiation positions. The zigzag tube shows necking before failure with some deformations in other places.

Keywords: Carbon nanotube, Stone-Wales defect, Mechanical property, Molecular dynamics simulation

1. INTRODUCTION

Fabrication of super strong composite materials can be realized in practice by the use of carbon nanotubes(CNTs) as reinforcing fibres. The choice of CNTs in these fields is found to be very much beneficial for their tremendous high strength and low density. But the prediction of their mechanical properties [1-3] often ends with some uncertainties especially due to some unavoidable defects produced in them during their production, purification or fictionalization. Stone-Wales (SW) defects [4], vacancies, pentagons, heptagons, lattice-trapped states, ad-dimers etc. are many types of defects that can appear in the CNT structure. Influence of defects can be observed in the mechanical properties of CNTs as well as electronic or magnetic properties. However, the effect of Stone-Wales defects have been investigated by many researchers [5-7] to obtain a clear understanding of their influence. A SW defect is produced by 90^0 rotation of a C-C bond and thus producing two pentagons and two heptagons. No matter what the process or potential adopted, reduction of failure strength and failure strain was reported by most of the authors. Adopting Brenner's bond order potential, Pozrikidis [8] has shown that inclined, axial and circumferential defect orientations have a strong influence on the mechanical response of zigzag and armchair single-walled carbon nanotubes (SWCNTs). Recently an attempt to explain the reason of scattering in data of the mechanical properties of CNTs has been made by Tunvir et al. [9] with Morse potential. To investigate the interference effect of spatial arrangements between two neighboring vacancy and SW defects with respect to the loading direction, their relative distances as well as their local orientations have been varied and the results compared. But they have considered the defects in the middle of a (10, 10) SWCNT and in only one side of the tube. The influence of odd and even number of SW defects are investigated in a recent study [10] by the present authors.

As the SWCNTs have cylindrical geometry, defects may lie on its surface in a particular spatial configuration. Keeping this in mind, more than one defect are considered at different positions of a zigzag (10, 0) SWCNT with varying separating distances and different angular orientations to simulate them in atomic scale. Tersoff-Brenner [11] potential is employed to represent the interaction of the C-C bond, which can explain adequately the creation and destruction of bonds in a CNT structure. Defects are distributed in all parts of the tube and moreover, diagonal, overlapping and neighboring defects are taken along with many other possible arrangements. Fracture modes are modeled and compared, with a detailed study of the mechanical responses of the tubes viz., Young's modulus, failure strength and ductility.

2. THEORETICAL METHOD

A zigzag (10, 0) SWCNT of length 49.19 Å is considered in this study. The basic pattern of 40 atoms is repeated in space to form the tube which contains 400 atoms as a whole. Berendsen thermostat [12] is used to allow small changes in the velocities of the atoms such that the temperature of the system reaches an equilibrium value close to 300K. The tube is stretched in the axial direction keeping the other end fixed. By stretching in small strain increments, the equilibrium potential energy is calculated by simulation, at first in absence of any defect, and then with 1, 2, 3 and 4 defects at different positions of the tube.

Stretch is applied along the axis of the tube. No other constraint is set up other than the condition that the force is zero in any other direction.

Stress is calculated from the energy-strain curve as $\sigma = 1/V\ (dE/d\varepsilon)$ where σ is the longitudinal stress, V the volume of the tube, ε the strain and E the strain energy of the tube. Volume of the tube is calculated as $V = 2\pi r \delta r l$ where r is the inner radius of the tube, δr its wall thickness and l the length of the tube. We have taken δr as 0.34 nm, which has been the standard value, used by most of the authors. To calculate stress from the energy-strain curve we have used a linear relationship for the elastic region and appropriate non-linear polynomial fit for the segments of high strain deformation regions. Young's modulus is found from the slope of the linear portion of the stress-strain curve. By changing the (z, r, θ) values, defects are created at different positions of the same tube. θ is changed by 90^0 from its first value to form two oppositely oriented defects. To produce two diagonal defects, θ is changed by 45^0 and z is adjusted to the desired value.

3. RESULTS AND DISCUSSION

3.1 Mechanical characteristics of a defect- free tube

In our calculation, the failure strength of a zigzag SWCNT is 115.4 GPa and maximum strain before failure is 18%. Young's modulus of the perfect tube is found to be 1.06 TPa [Fig 1]. Our calculation matches with the experimental values of failure stress by Demczyk [13] which is 150±45 GPa. Young's modulus is also close to the experimental value of 1.28 TPa by Wong et al. [14] and 1.25 TPa by Krishan et al.[15]. Maximum strain can be compared with the results of quantum mechanical calculations [6, 16] though 10-13% maximum strain and failure stress between 13-52 GPa were observed by Yu et al. [17]. For a pristine tube. several SW rotations are observed at strain above 10%.

3.2: Effect of a single defect

Young's modulus of the SWCNT is reduced by 24% by the inclusion of one defect. But ductility remains almost same. In maximum cases stress-strain curves are straight lines up to 7-8% strain. Strain energy (E_d) increases when a defect is introduced in the tube structure. Fig 1 below shows the stress-strain curves of a (10, 0) SWCNT with a single defect at different positions. Stress-strain curves [Fig 1] show the variation of the mechanical behavior of the tube mainly in the non-linear portion after inclusion of a single defect at different places. Failure stress is reduced to a maximum value of 103.59 GPa from its initial value. The results are tabulated in Table 1.

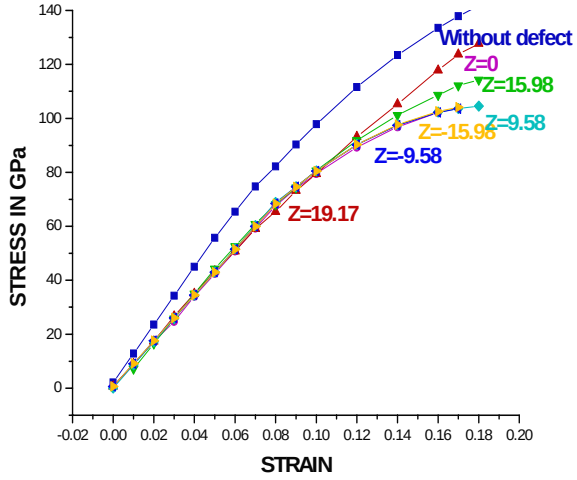

Fig 1: Stress-strain curves for a (10, 0) SWCNT with a single defect at different positions

3.3 Effect of a couple of defects

Interesting results are obtained with different combinations of two defects. Results are shown in Fig 2.

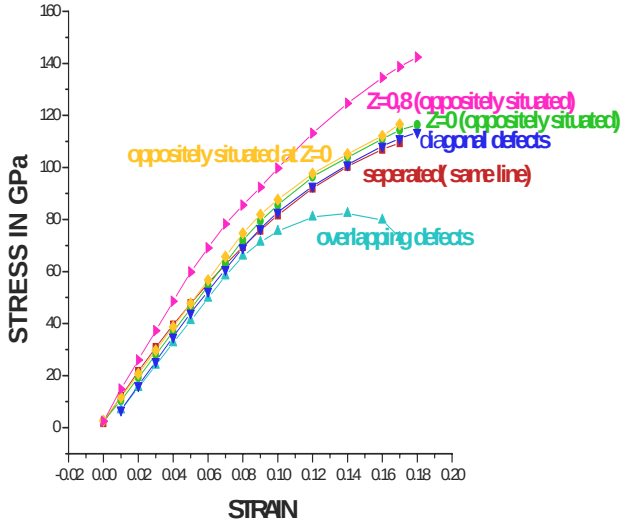

Fig. 2: Stress-strain curves for a (10,0) SWCNT with two defects at different positions

Tensile strength and Y value here are higher than the result of inclusion of one defect except for two diagonally situated defects and when the defects are situated on the same line separated by a distance. Defect-defect interaction [18] is different in each case. Repulsive interaction between defects is said to occur when failure strength is reduced greatly. But when this reduction is not much, we can say that the defects attract each other.

3.4 Influence of three defects

Different combinations of three defects are taken to study the effect of odd number of defects. An aggregation of three diagonal defects in a zigzag tube reduces the strength of the tube to 89.58 GPa.[Fig 3]. Reduction of strength is also remarkable when the defects are close and almost on the same line (orientation of one defect differs only by 9^0). Like two defects on the same line, three such defects exactly on the same line have no such pronounced effect on the tensile strength of the tube. The middle defect here is influenced in a complex manner by the other two defects. In each case, different results are obtained [Table 1]. For the defects that are oriented by some angle with respect to each other, the curvature plays a significant role in decreasing the strength. For defects on the same line, mainly the separation between the defects is important.

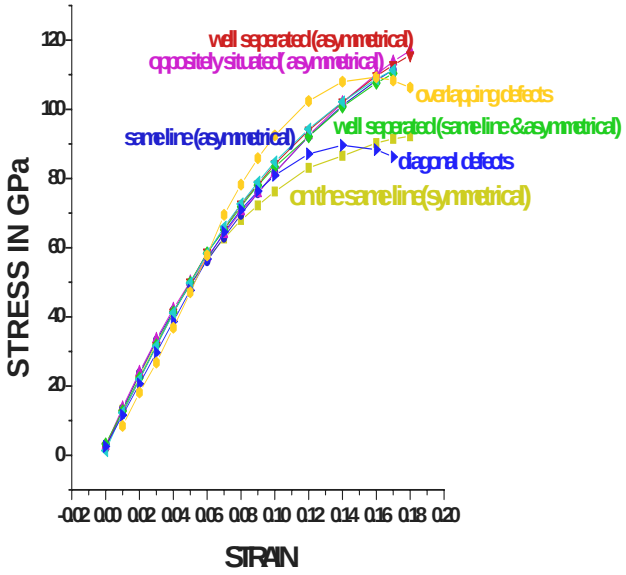

Fig 3: Stress-strain curves for a (10, 0) SWCNT with 3 defects at different positions

3.5 Results of inclusion of four defects

When four defects are placed asymmetrically on the same line in a zigzag (10, 0) SWCNT, the failure strength is very much reduced. 93.81 GPa is the lowest strength of the tube with four defects.

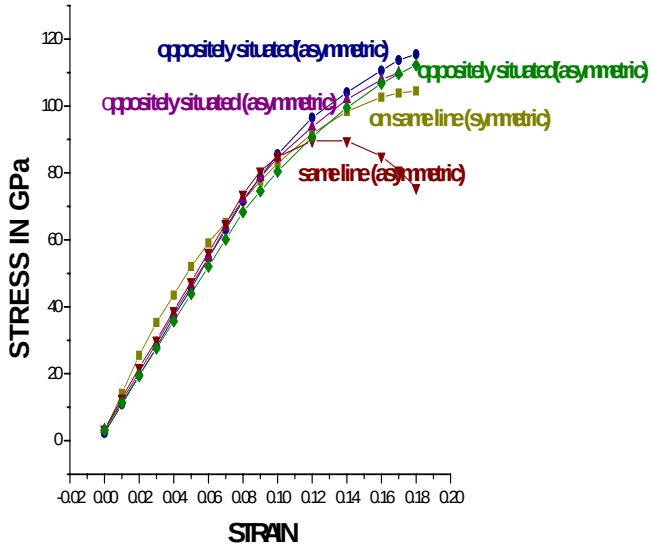

Fig 4: Stress-Strain curves of a (10,0) SWNT with 4 defects at different positions

3.6 Modeling of fracture behavior

Necking is observed before failure for the pristine tube. Fracture of a defect- free tube is shown in fig 5(a). Breaking of the tube with one or more defects sometimes [Fig 5(c, e, f)] show deformation of the tube in other places. With three diagonal defects [Fig 5(d)]the fracture of the tube is associated with several breaking of bonds. Fracture in no case is sharp. With four defects [Fig 5(f)] the tube does not break from any defect site.

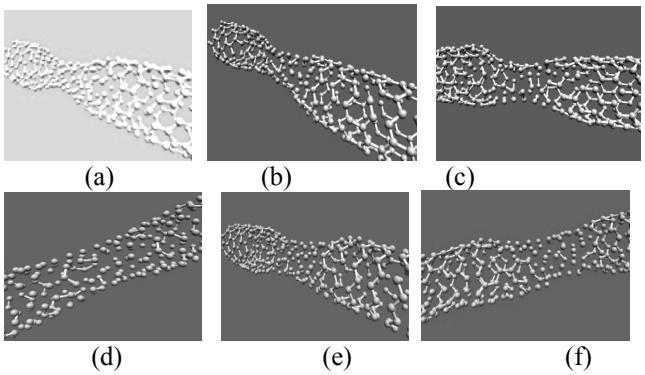

Fig 5: Breaking of a (10, 0) SWNT **(a)** without defect **(b)** with a single defect at (z, r, θ) position (15.98, 3.87, 9) **(c)** with 2 defects at (-1.06,3.87,-9) & (1.06,3.87,27) **(d)** with 3 defects at (0.00,3.91,90), (4.26,3.91,126) & (3.91, 3.87, 171) **(e)** (0.00,3.91,90), (-8.52,3.91,-90) & (-17.04.3.89, 90) and **(f)** with 4 defects at (-4.26, 3.91, 90), (12.78, 3.91, 90), (4.26,3.91,90) & (-12.78, 3.91,90)

	(z, r, θ) Position of defects	Y.M.* (TPa)	T.S.** (GPa)
1 DEFECT	(0, 3.91, 18)	.832	105.34
	(9.58, 3.87, 99	.859	104.66
	(-9.58, 3.87, 99)	.847	103.59
	(15.98, 3.87, 9)	.824	116.67
	(-15.98, 3.87, 9)	.846	104.14
	(19.17, 3.91, 36)	.821	127.71
	(-19.17, 3.91, 36)	.829	106.67
2 DEFECTS	(-4.26,3.91,54), (4.26,3.91,54)	.891	109.44
	(-4.26,3.91,90),(4.26,3.91,90)	.873	116.38
	(0,3.91,90), (8.52,3.91,-90)	1.00	141.7
	(-1.06,3.87,-9), (1.06,3.87,27)	.849	82.31
	(2.13.3.91,0), (0.00,3.91,90)	.893	113.5
	(0,3.91,-18), (,3.91,162)	.900	116.58
	(-3.19,3.87,27), (3.19,3.87,27)	.832	85.87
3 DEFECTS	(-4.26,3.91,99), (0.00,3.91,90),(4.26,3.91,90)	.904	92.19
	(0.00,3.91,90), (-4.26,3.91,90),(8.52,3.91,90)	.865	111.41
	(-4.26,3.91,-90), (4.26,3.91,90),(17.04,3.91,90)	.95	117.02
	(0.00,3.91,90), (-8.52,3.91,-90),(-17.04.3.89,90)	.94	115.6
	(0.00,3.91,90), (-8.52,3.91,90),(-17.04,3.91,90)	.924	110.36
	(0.00,3.91,90), (8.52,3.91,90)(17.04,3.91,90)	.946	111.28
	(0.00,3.91,90),(4.26,3.91,126),(3.91,3.87,171)	.892	89.58
	(0.00,3.91,90), (3.91,3.87,99),(7.45,3.87,99)	.898	109.28
4 DEFECTS	(-4.26,3.91,90), (12.78,3.91,90),(3.04, 2.65, 99), (7.45, 2.7, 90)	.74	93.81
	(-15.52, 2.65, 88), (-7.45, 2.73, 90),(7.45, 2.7, 90), (14.30, 2.65, 88)	.758	145.22
	(-15.52, 2.65, 88), (-5.02, 2.73, 97),(5.02, 2.73, -97), (15.52, 2.65, -88)	.756	88.09
	(-19.93, 2.7, 97), (-9.89,2.73, 83),(0.00,3.91,90), (4.26,3.91,90)	.792	98.92
	(-6.24, 2.7, 94), (-2.59, 2.73, 105)(0.61, 2.65, 92), (3.8, 2.73, 79)	.814	86.81

Table 1: Young's Modulus and Tensile strength of a (10, 0) SWCNT with defects at different positions
*Y.M.-Young's modulus, **T.S.- Tensile Strength

5. CONCLUSIONS

The mechanical properties of a (10, 0) SWCNT are influenced by the presence of SW defects. Their number, position, orientation and their arrangement are responsible for the changes in mechanical characteristics. The ductility of the zigzag tube is not influenced by the inclusion of defects. Results with more than one defect show defect-defect correlation. Neighboring defects, especially a combination of overlapping defects reduces the failure strength of the tube significantly. An increased number of defects do not show any marked influence on the mechanical properties of the nanotubes.

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