International Journal of Application or Innovation in Engineering & Management (IJAIEM)
Web Site: www.ijaiem.org Email: editor@ijaiem.org, editorijaiem@gmail.com
Volume 2, Issue 2, February 2013 ISSN 2319 - 4847

Molecular Dynamics Simulation Study of Novel Properties of Defect Full Single Walled Carbon Nanotubes

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ABSTRACT

Basis of the present study is comparative investigation of effects produced by Stone-Wales (S-W) and vacancy defects (VD) on the novel performance of single walled carbon Nanotubes (SWCNTs). The variation of defect is 1 to 4 in both VD and S-W. Molecular dynamics (MD) simulation has been used to generate the mechanical performance of SWCNTs. Simulations have been carried out on a 42.59Å long armchair (6, 6) and (10, 10) SWCNTs by varying their relative positions and orientations. Tensile strengths are reduced by an average value of 23.48% and 28.2% for 4 VD and 4 S-W defects respectively. The Young's modulus of pristine CNT is weakened by 9.38% and 11.23% for S-W defects and VD respectively.

Keywords: Single-walled carbon nanotube; Mechanical performance; Young Modulus; Molecular Dynamics; Stone Wales defect; Vacancy defect.

1. INTRODUCTION

Carbon nanotubes (CNTs) have attracted deep research interest due to their unique properties such as high stiffness against bending and high tensile strength [1]. Using CNTs as reinforcement material to enhance the mechanical properties of composite materials has been pursued extensively in both experimental and theoretical studies. Defected CNTs play vital role in decreasing the mechanical strength of the composites and S-W as well as VD have received considerable attention. Using CNTs as reinforcing agents to design and fabricate strong composites with desirable mechanical properties needs thorough understanding of the mechanical behavior of such nanotubes. In recent years, mechanical, thermal and electrical properties have spurred considerable interest among researchers and as a result many experimental and theoretical studies have been performed so far to explore these remarkable mechanical properties CNTs [2, 3] have shown their high potential in improving the material properties of polymers. Computer simulations are increasingly used to guide experimentalists in interpreting the results and even to reduce some of the laboratory tests. However, as with any other man-made products, CNTs were also found to be susceptible to defects. Belytschko et al. [4] have used molecular mechanics approach on Morse and Brenner potentials to study the fracture of a CNT. They observed that even a single missing atom can reduce its strength by about 25%. Zhang et al. [5] have investigated the effects of one and two atomic vacancy defects, slits and holes on the fracture of SWCNTs, double-walled CNTs(DWCNTs) and triple-walled CNTs (TWCNTs) using atomistic simulations and multi-scale methods.
The aim of this study is to make the comparison between the mechanical properties of CNT obtained by deliberately introduced S-W and vacancy defects by using the MD simulations. Both the defects have been classified into two basic types; they are one and four for both vacancy and S-W defects. The study has been focused on the calculations and comparisons of tensile strengths and strain of various chiralities SWCNTs with inclusion of number of vacancy and S-W defects. The results obtained by the inclusion of both defects have been compared with mechanical properties obtained from pristine CNTs. Young's modulus of defected CNTs have also been calculated by increasing the lattice size thereby decreasing the density. The potential energy calculation has been made to calculate the energy required to stabilize the structure of different chiralities CNTs.

2. DEFECT FORMATION

2.1. Stone-Wales Defect

To create S-W defect, four neighboring hexagons are converted into two pentagons and two heptagons with a 90_0 rotation of the horizontal bond of the hexagonal structure [12], as shown in figures 1 and 2. In case of 1 S-W defect, the defect has been placed at the middle of the CNT structure whereas in case of 2, 3 and 4 S-W defects, the defects have been placed equidistant, as shown in the schematic and computer constructed models in Figures 1 and 2.

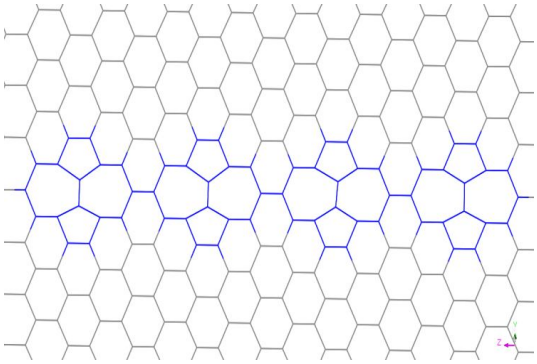

Fig. 1 Schematic of S-W defects with defect densities four

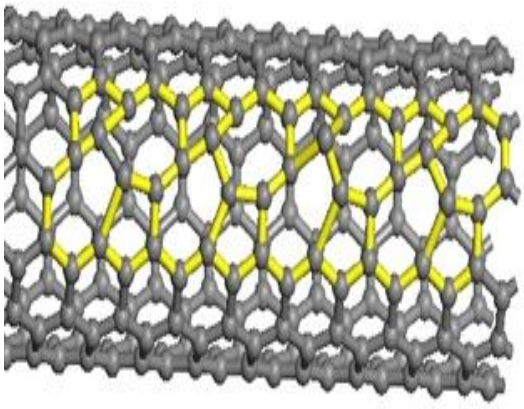

Fig. 2: Computer constructed S-W defect with defect densities four

The various transformations involved in the conversion of 4 hexagons to 2 pentagons lead to elongation of the structure along the axis connecting the pentagon's and shrinkage along the perpendicular direction. Thus, the rotation of the bond from a predominantly circumferential to predominantly axial orientation lengthens the tube but not to such an extent to change the load distribution between the bonds in the nanotube. For the sake of simplicity, it has been assumed that after the creation of S-W defect, the dimension of the nanotube remains unchanged. Beyond a critical level of tension, CNT releases its excessive strain through a spontaneous formation of topological defects. It has been proposed that at high temperatures, a plastic response could occur due to the separation and gliding of S-W defects, whereas at lower temperatures the result could be fractures. The orientations of all S-W defects from 1 to 4 have been taken in the same vertical line.

2.2 Vacancy Defect

To create VD defects, carbon atoms have been removed from the perfect hexagonal structure of the CNTs creating a vacancy at the place of missing atom as shown in Figures 3 and 4. If a single atom is removed from the lattice, its three neighbours will become less stable because their sp^2 bonds are not saturated. Any two of these carbon atoms can be reconnected to form a new bond as shown in figures 3 and 4. A two atom vacancy defect is modeled by taking out two adjacent carbon atoms followed by bond reconstructions. When the two adjacent carbon atoms forming one c=c sp^2 bond, are taken out, the four neighboring atoms become unsaturated.

A four atom or cluster vacancy defect is created if more than 3 carbon atoms are taken out at one location, generating a hole or crack. Since the numbers of missing atoms are larger than three, there may be many possible configurations during the bond reconstruction. This study, considers connecting the 2 unsaturated atoms that are neighbours of the same missing atoms, as shown in Figures 3 and 4. In case of 1 vacancy defect the other 2, 3 and 4 vacancy defects have been placed at equal distance from the defect at the middle. It has been observed that the orientations of all four defects are in the same vertical line.

2.3 Energy Optimization

The structure of carbon nanotube is identified by using the nomenclature (n, m) [13]. The present study focuses on armchair tubes with some values of "n" and "m" equal to 6 and 10. The accuracy of the MD models has been increased by applying periodic boundary conditions. Periodic and super cells for different SWCNTs (Pristine along with 1 and 4 VD and S-W defects) are built by using the material studio software. By applying the periodic boundary conditions, the effect of bulk environment can be created within this unit configuration, which improves the accuracy of the MD models. A super cell is built with 10 repeated units in the Z-direction to achieve the length of SWCNT equal to 42.59Å and diameter 3.92Å (i.e. aspect ratio 10.87). The major reason of making the super cell in Z- direction is to identify the elastic modulus in the axial direction of the nanotube from elastic constant matrix.

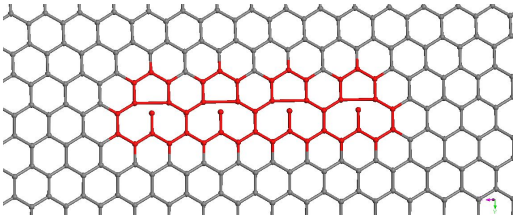

Fig. 3 Schematic of Vacancy defect with defect densities four

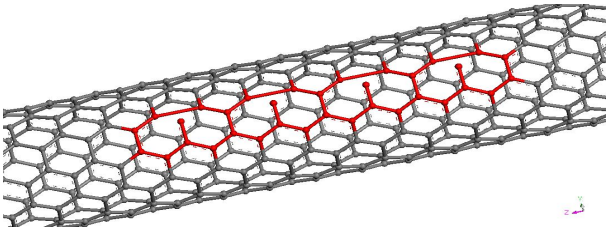

Fig. 4 Computer constructed Vacancy defects with defect densities fourMethodology

The lattice parameters have been assigned with all the angles as 900 to achieve a periodic box around the CNT. The lattice size has been assigned in terms of "a=23.628", "b=23.628" and "c=24.595" in x, y and z direction respectively. Once the lattice parameters have been set, the potential as well as the non-bond energy is minimized to get the stabilized structure. In this study, this has been achieved with the help of Discover minimization using Steepest descent method with 5,000 no's of iterations, whereas the convergence rate is 0.1 k/cal/mol/Å.

2.4 MD Simulations

The condensed-phase optimized molecular potential for atomistic simulation studies (COMPASS) force fields have been used in the simulation. The COMPASS force field enables accurate and simultaneous prediction of mechanical, structural vibration and thermal properties accurately for a large range of molecules in isolation and in condensed phase under a wide range of conditions of temperature and pressure. Following the energy minimization, MD simulations are carried out at room temperature (298 K) using the ensembles of constant number of particles, constant volume and constant temperature (NVT).

All the simulations are performed with an interval of 1 femtosecond (fs) in each MD simulation step. The thickness of the graphene sheet has been taken as 0.34Å. For each kind of MD model, velocities of atoms in each region are averaged over last 1 ps period to the temperature calculation along the SWCNT. Ten repeated units have been taken of the original SWCNTs (6, 6) and (10, 10) which contain 288 atoms. Though the SWCNTs considered in this study have small length, having an aspect ratio greater than 10, the results will not be affected by any end effect. Stress has been calculated from the energy value according to the relation $\sigma = 1/A(\partial E/\partial \epsilon)$ where σ is the stress, A is the area of the annular cross-section of the tube, $(\partial E/\partial \epsilon)$ is the slope of the energy curve and Є represents the strain.

3. RESULTS AND DISCUSSIONS

Figures 5 and 6 show the variation of stress and strain induced in SWCNTs in both the cases of S-W and VD. The trends of variation of stress and strain are the same for all different bond length nanotubes. With the presence of 1 and 4 VD, tensile strength of the nanotube reduces by 23.23% and 23.48 on an average, respectively, and tensile failure strain reduces by 20.7% and 24.4% on an average, respectively

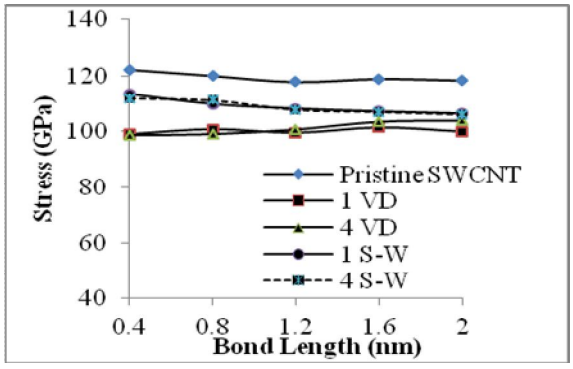

Fig. 5: Tensile failure strengths of different pristine and defective SWCNTs

For different bond lengths However, in case of S-W defect this reduction in strength (strain) is only 7.45% (25.8%) and 8.92% (29.2%) for 1 and 4 defects, respectively. It is seen that for the same defect density, VD reduces the tensile strength of nanotubes much more then S-W defect does. This happens because such type of defects creates hole or void in the nanotubes at which failure of the tubes can easily start.

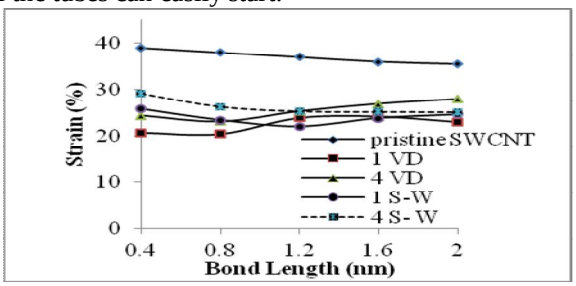

Fig. 6 Tensile failure strains of different pristine and defective SWCNTs

The potential energy curves of pristine SWCNT along with defective SWCNTs have been shown in Figures 7 and 8. Potential energy has been considerably increased due to the presence of defects in the nanotubes. For a particular type of defect, increase in the potential energy is almost same for 1 defect but a considerably large change has been noticed with the increase of defect densities (i.e. number of defects). It has been observed that with the presence of 1 and 4 vacancy defects, potential energy has been increased by 2.03% and 13.4%, respectively. However, in case of S-W defect, the increase in potential energy has been 4.4% and 21.1% for 1 and 4 defects, respectively.It may be noted that S-W defect has the greater effect on the performance of SWCNTs; it means that higher values of potential energies are required to stabilize the structure in the CNTs having S-W defects. It is concluded that the VD changes the bonding configuration of the SWCNT more than S-W effects. Due to this, increase of the potential energy is required to stabilize the individual SWCNT structure.

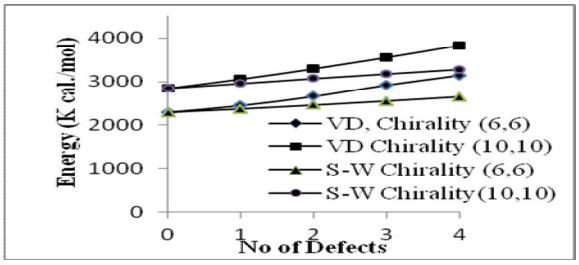

Fig. 7 Comparative study of Energy vs. No. of defects with respect to pristine SWCNTs

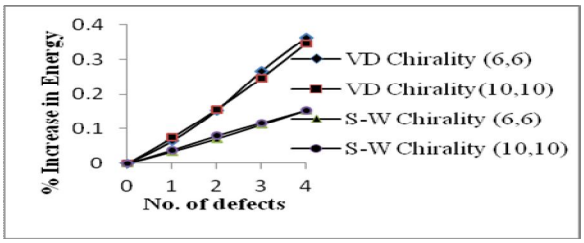

Fig. 8 Comparative study of Total Energy vs. No. of defects with respect to pristine SWCNTs

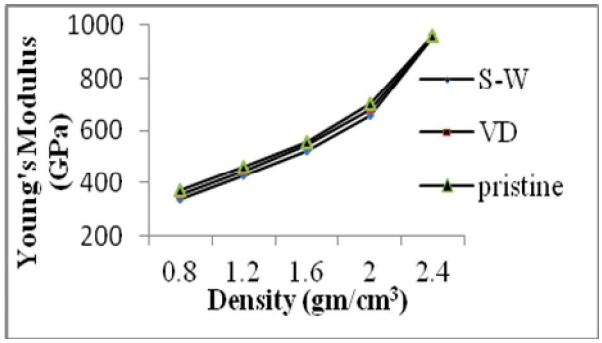

Fig. 9: Comparative study of Young's Modulus vs. Density of pristine and defective SWCNTs

Variations of Young's modulus with density of defected SWCNTs have been shown in figure 9 and it is observed that the Young's modulus increases as the density increases. The increase in density can be achieved by increasing the lattice size. A simple but effective observation can be made that the effect of different defects decreases as density increases. Hence the Young's modulus of SWCNTs increases. It can easily see from the table 1 and figure 9 that the percentage difference has been decreases from 9.38 to 0.4 and 5.09 to 0.9 in both cases S-W and VD respectively.

Table 1:- Variation of Young's modulus with density

Density (gm/cm3)	Young's Modulus (GPa)			% Difference	
	pristine	S-W defect	VD	S-W defect	VD
0.8	373.7086	338.139	354.89	9.38	5.09
1.2	458.6232	424.78	442.329	7.37	3.55
1.6	555.6935	524.574	542.261	5.6	2.41
2	699.6232	679.2937	689.015	2.86	1.43
2.4	960	956	951	0.4	0.9

4. CONCLUSION

The novel properties of armchair SWCNTs are greatly influenced by the inclusion of vacancy defects as compared to Stone-Wales defects. Their number, position, orientation and arrangement are responsible for the changes in mechanical characteristics. An increasing number of neighboring defects show a remarkable influence on the mechanical properties of the nanotubes. The following conclusions have been drawn:

- Presence of defects substantially reduces the tensile strength. In general, novel properties seem to decrease as the number of defects increases. This could be due to bond-bond interactions or due to chemical instabilities of the defects.
- Failure strain increases with the increase of defect density.
- More potential energy is required to stabilize the different structure of SWCNTs after inclusion of different defect densities as compared to the pristine CNTs. It is also noticed that requirement in the potential energy increases with the chiralities of the SWCNTs.

Presence of different defects decreases the performance of SWCNTs. These problems may overcome by increasing the lattice size and hence the density. This can also help to save the SWCNTs from distortion, consequently which reduces the overall strength of the composites. It is noticed that the effect of different defects decreases as density increases.

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