Available online at www.sciencedirect.com

ScienceDirect

Procedia Technology 23 (2016) 114 – 121

Procedia Technology

3rd International Conference on Innovations in Automation and Mechatronics Engineering, ICIAME 2016

Prediction of fracture pattern in defective Single walled carbon nanotubes using Molecular Structural mechanics

Ajay Patel[a*], Bhavik Ardeshana[b], Umang Jani[c], Anand Joshi[d]

[a,b,c,d]*Mechatronics Department,G.H.Patel College of Engineering and Technology, Vallabh Vidhyanagar, Gujarat-388120, India*

Abstract

An atomistic-based dynamic crack model for recreating execution of carbon nanotubes by considering vacancy defects is projected. The idea of the fracture model is taking into account the supposition that carbon nanotubes, when stacked, carry on like space-casing structures. The finite element method is utilized to analyse the nanotube structure and the molecular structural mechanics approach with beam element is used to simulate the non-linear force field of the C–C bonds. The model has been applied to defected single walled chiral, arm chair and zigzag nanotubes subjected to critical tension. The defect presented here (model) is one absent atom at the centre of the nanotube. The anticipated crack advancement, failure stresses of the nanotubes correspond exceptionally well with sub-atomic mechanics model from the literature.

Peer-review under responsibility of the organizing committee of ICIAME 2016

Keywords: SWCNT, Fracture pattern, Finite Element Analysis (FEA), Carbon nanotube

1. Introduction

Carbon nanotubes (CNTs), because of their remarkable mechanical properties, have animated incredible hobby and broad examination with respect to the estimation of their definite mechanical properties and quest for potential basic applications since the time that their innovation by Iijima [1].

*Ajay M. Patel. Tel.: +91-942-703-7011; fax:+0-269-223-6896.

E-mail address:ajaympatel2003@yahoo.com

Peer-review under responsibility of the organizing committee of ICIAME 2016
doi:10.1016/j.protcy.2016.03.006

Particular attributes, for example, the amazingly high stiffness and strength, which are in the scope of TPa, the amazing versatility, the capacity to maintain huge flexible strain and additionally the high angle proportion and low thickness make CNTs the perfect fortifying material for another class of super strong Nano-composites [2]. Other than the utilization of CNTs as customary carbon strands for fortifying polymer grid, a few potential applications have been of late investigated. Amongst them, is the utilization of CNTs for enhancing the out-of-plane and interlaminar properties of presently utilized propelled composites and their arrangement opposite to breaks so as to back off the make development by crossing over laugh hysterically the split appearances [3, 4].

The powerful utilization of CNTs in basic applications relies on upon their mechanical execution as stand-alone units. Test observation have uncovered that topological deformities, for example, the Stone–Wales imperfection and opening deformities, are usually present in CNT[5]. Imperfections corrupt the mechanical execution of CNTs, since they change their inelastic properties as well as the flexible, for example, the Young's modulus and Poisson's proportion. The longitudinal and transverse stiffness's and also the flexural unbending nature in strain, torsion and bowing are, thus, being adjusted. For instance, Chandra et al. [6] have demonstrated that the vicinity of Stone–Wales deformity lessens the firmness of the deserted region by around 30–50% bringing about decrease of the nanotube Young's modulus. Mechanical properties and distortion of CNTs have been broadly considered amid the most recent couple of years both tentatively and hypothetically. From the perspective of hypothetical displaying, two methodologies have been basically received: the atomistic methodologies (Classical molecular Dynamics (MD) and mechanics (MM)) and the continuum mechanics approaches. In the larger part of studies, CNTs have been reproduced as deformity free materials dismissing both the impact of starting imperfections and in addition the impact of any conceivable breaks that may show up amid stacking. Belyschko et al. [7], Mielke et al. [8], Liew et al. [9] are perform the MM and MD simulation done for finding the mechanical preformation of CNTs by considering such effect. Chandra et al. [6], measure the stress and strain at the atomic scale. Belyschko et al. [7] have finding the fracture of CNTs by taking the MM simulation, under the axial tension. They originate the fracture is nearly independent on the separation energy and depend on the inflection point of the interamotic potential. The zigzag nanotube have failure strain around 10 to 15% based on the prediction, and compare with experiment result. As well as failure stress was found around 65-93 GPa, which was higher than the experiment. The facture of the CNTs with vacancy defects and under axil tension was explore by the Mielke et al. [8] using the quantum mechanics calculation with density function theory and MM calculation done with Tersoff-Brenner potential and semi empirical methods. All these methods give suitable result which is comparable with experiment. This is partly due to the fact that the majority of researchers have adopted continuum shell models, which treat CNTs as continuum hollow cylinders being unable to consider defects, and therefore, fracture. Progressive fracture model is proposed, satisfies these requirements. Patel and Joshi [10] investigated the mass recognition characteristics of double walled Carbon Nanotubes using analytical and Finite Element Procedure. Patel and Joshi [11-13] have been investigated resonant frequency and frequency shift of double walled carbon nanotubes with deviances along it is axis and different types of boundary conditions i.e., cantilever and bridged. The sensitivity of the actually turned double walled carbon nanotubes, different masses attached to the end of outer tube tip on DWCNT and centre outer tube tip of the bridged DWCNT and different lengths has been discovered and presented. In this paper, an atomistic- based progressive fracture model is considered for Finite Element Analysis (FEA).

Nomenclature

E	Potential Energy of Nanotube
$E_{stretch}$	Bond Energy due to bond Stretching
E_{angle}	Bond Energy due to bond angle-bending
r	Current bond length
θ	Current angle the adjacent bond

2. Methodology

Atomistic- based continuum mechanics approaches developed for CNTs which is used to analyse the structural of CNTs, which defines the performance of C-C binds. Li and Chou [14] are the first to suggest such an approach. For

modelling of the bonds, they have used the stiffness matrix method, which are studied as space frame structure, and linked with molecular and structural mechanics to find the sectional property factors of beam members. Li and Chou [14], Teserpes and Papanikos [15] have established a finite element model for SWCNTs. Li and Chou [14] have proposed that the C-C bonds perform linearly and have used beam elements to represent bonds with constant Young's modulus. To simulate the performance of CNTs under large stresses C-C bonds must be model by empirical intertomatic potentials. To understand the fracture in CNT, a model has been proposed which considering the nonlinear performance of C-C bonds as explained by Teserpes and Papanikos [15]. Mechanical properties of CNTs were grounded by the Xiao et al. [16], stiffness and strength of SWCNTs were grounded by Sun and Zhao [17].

2.1 Algorithm of the model

The Model of C-C bonds has been created in Ansys using 3D elastic beam4 element. The non-linear performance of the C-C bonds as defined in interatomic potential, was assigned to the beam element of the model. The initial stiffness is 1.16 TPa. A constant amount of pressure is applied at one of the each ends and other end is kept fully constraints. Force was only applied in one direction, so buckling of Nano tube can be avoided at very high stress and after the breaking of bond. Figure 1 shows the carbon nanotube (14,0) model with exact boundary condition and applied loading condition. Force of 1 KN is applied on the one end side of the nano tube. One carbon atom is removed from the nano tube give an initial defect. After doing the analysis of the nano tube at given boundary condition and force, max principle stress in the direction of applied force is found from the report of the result. Then after bond has been removed from the original Nano tube model as per the value of max. Principle stress produced in the C-C bond. After removing one bond again above analysis process is continued until catastrophic failure of the nano-tube take place. The choice of this nano tube is made for verification propose to already available result in literature.

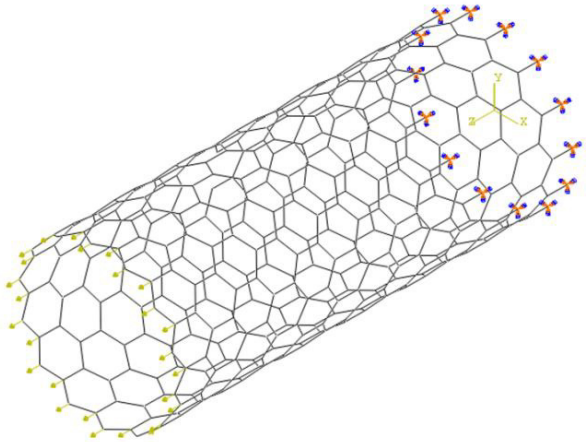


Fig. 1. FE mesh of the (14,0) tube with boundary condition and loading conditions

3. Molecular structural mechanics

In this paper, for utilizing the finite element procedure potential energy is used to evaluate linear nanospring stiffness. The total force on each atomic nuclei is the sum of the force generated by the electrons and electrostatics force between the positively charged nuclei themselves. The general formula for the potential energy is

$$U = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_\omega \quad (1)$$

Where, U_r is the energy due to bond stretch interaction, U_θ the energy due to bending (bond angle variation), U_Φ the energy due to dihedral angle torsion, U_ω the energy due to out-of-plane torsion.

$$U_r = \frac{1}{2}k_r(r-r_0)^2 = \frac{1}{2}k_r(\Delta r)^2 \quad (2)$$

$$U_\theta = \frac{1}{2}k_\theta(\theta-\theta_0)^2 = \frac{1}{2}k_\theta(\Delta\theta)^2 \quad (3)$$

$$U_\tau = U_\phi + U_\omega = \frac{1}{2}k_\tau(\Delta\phi)^2 \quad (4)$$

Where k_r, k_θ, and k_τ are the bond stretching, bond bending and torsional resistance force constants, respectively, while Δr, $\Delta\theta$ and $\Delta\emptyset$ represent bond stretching increment, bond angle variation and angle variation of bond twisting, respectively. In contrast to the other bonded interactions, the van der Waals interactions and the electrostatic forces may be neglected due their minor effects in terms of predicting the dynamics response of CNTs.

Molecular structural mechanics approach, there is a relationship between the sectional stiffness parameters in structural mechanics and the force constants in molecular mechanics. For convenience, the sections of carbon-carbon bonds are assumed to be identical and uniformly round like rods. Thus it can be assumed that Ix=Iy=I_Z and only three stiffness parameters, EA, EI and GJ, need to be determined.

As the potential energy in the two approaches are independent, energy equivalence of the stored energy of the two approaches, i.e. molecular mechanics and structural mechanics reveals [18].

$$\frac{EA}{L} = k_R; \qquad \frac{EI}{L} = k_\theta; \qquad \frac{GJ}{L} = k_\phi; \quad (5)$$

The elastic properties of the beam element are given as [19]

$$d = 4\sqrt{\frac{k_\theta}{k_R}}; \qquad E = \frac{{k_R}^2 L}{4\pi k_\theta}; \qquad G = \frac{{k_R}^2 k_\phi L}{8\pi {k_\theta}^2}; \quad (6)$$

Where, d, L, E and G represent the diameter, length, Young's Modulus and Shear Modulus of the beam element.

The second derivatives of the potential energy terms in Equations (2)-(4) with respect to bond length, bond angle and twisting bond angle variations produce the spring stiffness coefficients kr, kθ and k_τ according to Castigliano's theorem. The angle bending interaction is simulated with an axial nanospring, using the simplification described in [20]. The stiffness Ks of special spring is defined by following equation:

$$K_s = \left(\frac{1}{a_{c-c}\cos(60)^0}\right)^2 k_\theta \quad (7)$$

The angle may be varying for each C-C-C microstructure in a CNT according to its type and radius, due to cylindrical shape.

4. Initial defect

As specified in introduction, experimental observations have discovered that vacancy defects, introduced throughout the synthesis process, are usually present in CNTs. The very big difference between theoretical and experimental result of the young modulus and tensile strength of carbon nano tubes might be the amount of the defect present in the CNTs. Very little is known about the types of defect that has been developed during the synthesis process. Most likely defect is vacancy defects like missing atom.

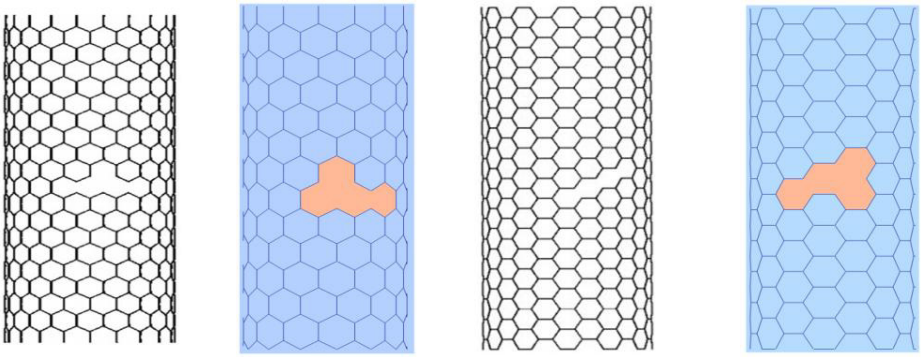
The fracture model is able to consider the two types of defect like topological and vacancy defects. The defect is created by removing one atom from anywhere on the topology of the FE model of CNT. Necessary modification was done on the FE model of the CNT.

In this paper the CNTs on which the fracture analysis has been done are taken from the literature. Only one type of defect is considered i.e. removal of one carbon atom and three bonds related to it. This defect was created in the middle of the CNTs.

5. Evaluation of Fracture

In this paper we are predicting the evaluation of fracture of the three types of CNTs as the same type of boundary condition and force. Fracture pattern of (14,0) zigzag CNT is compared with the literature of P. Papanikos' fracture pattern of (20,0) zigzag CNT. While other CNTs (8,8) and (13,2) are used to compare the effect of chirality of SWCNT on the strength or fracture of SWCNTs.

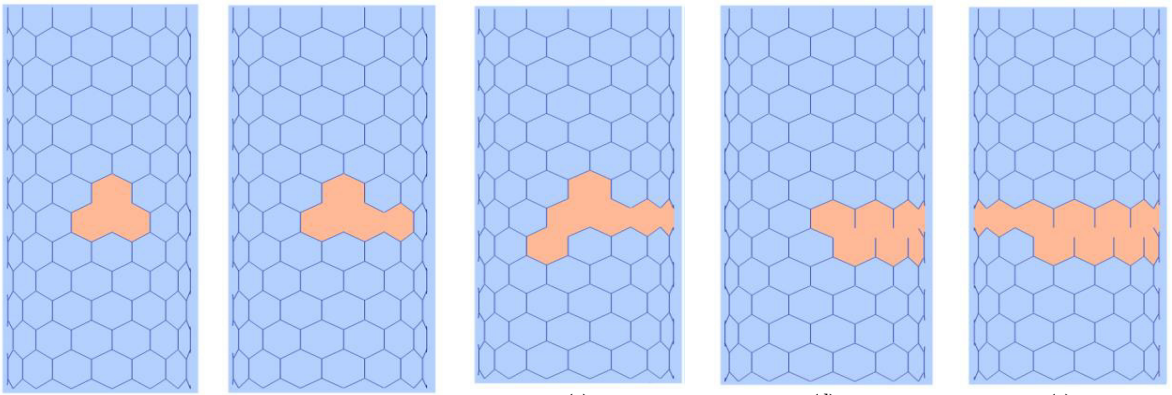
To verify the model, two different type Zigzag and Armchair SWCNT, the authors have compared the present model results with Tserpes and Papanikos [21]. Figure 2 shows Predicted fracture evolution in the Zigzag CNT (20,0) [21] and (14,0) present model, Armchair CNT (12,12)[21] and (8,8) present model, same evolution of fracture has been obtained for the same type of CNT. PFM was applied to zigzag (14,0), armchair (8,8), and chiral (13,2) nano tubes and numerical results were calculated and it was compared with the results of Tserpes and Papanikos [21] predictions.



CNT(20,0)[21] CNT(14,0) Present Model CNT(12,12)[21] CNT(8,8) Present Model

Fig. 2. Predicted fracture evolution in the Zigzag CNT (20,0) [21] and (14,0) present model, Armchair CNT (12,12)[21] and (8,8) present model.

Figure 3 shows the evolution of fracture of C-C bonds as the result of the force applied and affecting the different bonds one after another bonds. Figure 3 (a) shows the defective SWCNT with the three missing bond before loading. As may be seen from other figures that fracture propagated circumferentially at the same row without spreading into other rows while fracture started on the one direction of the surface but after some of the bonds removed in this direction then fracture again started from the opposite direction from the initial defect and both met at the opposite side of the cylindrical SWCNTs.



(a) (b) (c) (d) (e)

Fig. 3. Predicted fracture evolution in the (14,0) tube containing three missing bond and one atom; Parts (a), (b) and (c) of the fig show the evolution of fracture in the front half of the CNT, parts (d) and (e) in the back.

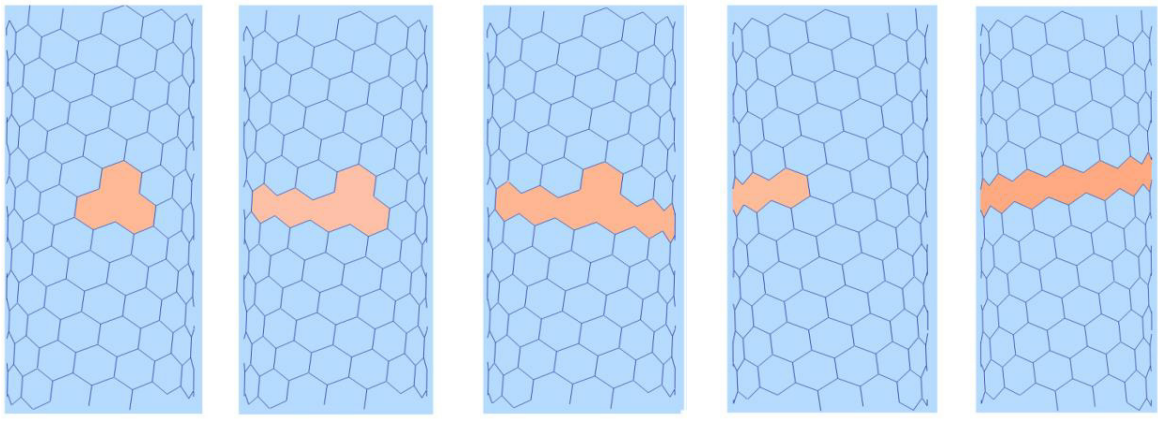


Fig. 4. Predicted fracture evolution in the (13,2) tube containing three missing bond and one atom; Parts (a), (b) and (c) of the fig show the evolution of fracture in the front half of the CNT, parts (d) and (e) in the back.

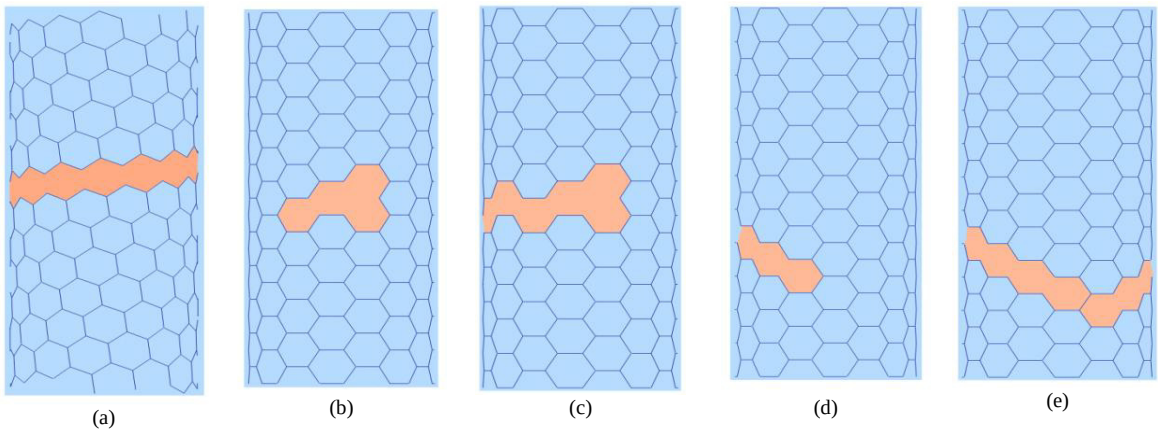


Fig. 5. Predicted fracture evolution in the (8,8) tube containing three missing bond and one atom; Parts (a), (b) and (c) of the fig show the evolution of fracture in the front half of the CNT, parts (d) and (e) in the back.

In the analyses performed, the stress produced in the last bond before the catastrophic failure is highest compared to other values of stress in different bonds that was removed in earlier stage of analysis.

Figure 4 shows the development of fracture in the (13,2) CNT which is same as the fracture of the (14,0) tube. But in case of (14,0) bonds break in continuously on the circumferential line perpendicular to the axis of CNT while in case of (13,2) bond break is repeatedly but line is not perpendicular to the axis of CNT. Figure 5 shows that armchair (8,8) carbon nanotube bond breaking sequence is diagonally. The reason of the type of failure can be attributed to the change in the stiffness values that take place when the type of CNT changes, i.e. armchair, chiral and zigzag. Along with the change in the type of CNT the orientation of the bond changes due to the change in the chiral angle which further changes the stiffness and hence the breakage pattern.

6. Results and Discussion

Number of steps taken by the CNTs before the catastrophic failure are 21 for (14,0), 16 for (13,2), and 18 for (8,8). From this values we can say that no. of bonds breaking before catastrophic failure is more in (14,0) than other SWCNT. The geometrical features of this CNTs are shown in Table 1. Figure 6 shows that Stress vs. Number of bond eliminate of chiral, Zigzag and Armchair CNTs. Eliminating of equal bond of three CNTs after that Chiral CNT(13,2) has minimum stress its indicate chiral CNT has better strength. Table 2 shows Stress value of eliminate bond of Chiral CNT (13,2) , Armchair CNT (8,8) and Zigzag(14,0). Its shows maximum stress value of zigzag CNT.

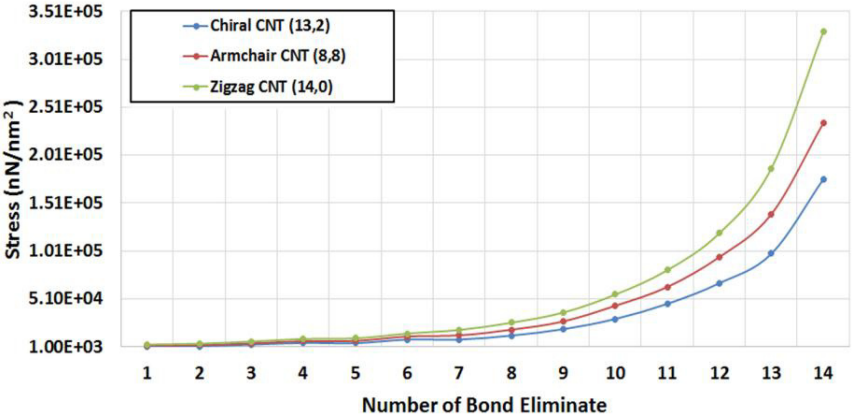


Fig. 6 Stress vs. Number of bond eliminate of three different type of CNTs

Table 1. Geometrical characteristics of SWCNTs

SWCNT	Length, Lo (nm)	Diameter, D (nm)	Number of atoms
(14,0)	34.23	10.89	533
(8,8)	33.88	10.78	524
(13,2)	34.50	10.98	528

Table 2 Stress value of eliminate bond of three different type CNT

Chiral (13,2)		Zigzag (14,0)		Armchair(8,8)	
Element Number	Stress (nN/nm^2)	Element number	Stress (nN/nm^2)	Element number	Stress (nN/nm^2)
246	1.47E+03	299	1.08E+03	359	1.05E+03
247	1.90E+03	300	1.54E+03	343	1.04E+03
244	3.53E+03	311	1.82E+03	311	1.35E+03
243	5.32E+03	310	2.33E+03	310	1.76E+03
228	5.02E+03	323	2.69E+03	309	2.36E+03
248	8.77E+03	309	3.05E+03	308	3.22E+03
249	8.80E+03	288	5.61E+03	307	4.38E+03
250	1.30E+04	303	7.25E+03	426	6.12E+03
251	1.96E+04	317	9.26E+03	448	8.09E+03
252	3.02E+04	304	1.17E+04	484	1.38E+04
253	4.60E+04	305	1.75E+04	177	1.76E+04
254	6.76E+04	292	2.48E+04	240	2.73E+04
255	9.82E+04	293	4.78E+04	306	4.13E+04
270	1.76E+05	294	9.55E+04	273	5.86E+04

7. Conclusion

The present work has analyzed the modeling of zigzag, armchair and chiral SWCNT using a finite element model. Evaluation of fracture of the three types of CNTs as the same type of boundary condition and force. The following conclusions are drawn from the study

- The model has been applied to defected single walled chiral nanotubes subjected to pivotal tension.
- Catastrophic failure are 21 for zigzag (14,0), 16 for armchair (8,8) and 18 for and chiral (13,2). It shows that zigzag (14,0) SWCNT more catastrophic failure compared to armchair and chiral.
- The failure pattern is found to be different in all the three types of SWCNTs mainly because of the orientation of the covalent bond between carbon - carbon atoms. This orientation further leads to the change in the stiffness of the bonds which further leads to increase in the stress at the junction and later on failure of the tube.
- Chiral CNT (13,2) has better strength compare to Armchair (8,8) and zigzag (14,0).

Acknowledgements

The authors would like to acknowledge the DST grant no. SB/FTP/ETA-106/2013, provided by Department of Science and Technology (DST), Science and Engineering Research Board, Govt. of India.

References

[1] Iijima S. Helical microtubules of graphitic carbon. Nature 1991; 354:56–68.
[2] Lau K-T, Hui D. The revolutionary creation of new advanced materials–carbon nanotube composites. Compos Part B Eng 2002; 33:263–77.
[3] Lau K-T, Hui D. Effectiveness of using carbon nanotubes as nano-reinforcements for advanced composite structures.Carbon 2002; 40:1605–6.
[4] Qian D, Dickey EC, Andrews R, Rantell T. Load transfer and deformation mechanisms in carbon nanotube-polystyrene composites. Appl Phys Lett 2000; 76(20):2868–70.
[5] Ebbesen TW, Takada T. Topological and sp3 defect structures in nanotubes. Carbon 1995; 33(7):937–78.
[6] Chandra N, Namilae S, Shet C. Local elastic properties of carbon nanotubes in the presence of Stone–Wales defects. Phys Rev B 2004; 69:094101.
[7] Belytschko T, Xiao SP, Schatz GC, Ruoff RS. Atomistic simulations of nanotube fracture. Phys Rev B 2002; 65:235430.
[8] Mielke SL, Troya D, Zhang S, Li J-L, Xiao S, Car R, et al. The role of vacancy defects and holes in the fracture of carbon nanotubes. Chem Phys Lett 2004; 390:413–20.
[9] Liew KM, He XQ, Wong CH. On the study of elastic and plastic properties of multi-walled carbon nanotubes under axial tension using molecular dynamics simulations. Acta Materiala 2004; 52:2521–7.
[10] Ajay M. Patel, Joshi A.Y., 2013, "Vibration Analysis of Double Wall Carbon Nanotube based Resonators for Zeptogram level Mass Recognition", Computational Materials Science, Elsevier Publishers, Volume 79, , Pp 230–238.
[11] Patel Ajay M., Joshi A.Y., "Investigating the Influence of Surface Deviations in Double Wall Carbon Nanotube based Nanomechanical Sensors", Computational Materials Science, Volume 89, April 2014, Pages 157–164.
[12] Ajay M. Patel, Joshi A.Y. 2014 "Effect of Waviness on the Dynamic Characteristics of Double Walled Carbon Nanotubes" Nanoscience Nano technology Letter, vol- 6, 1-9.
[13] Ajay M. Patel, Anand Y Joshi, "Influence of atomic vacancies on the dynamic characteristics of nanoresonators based on double walled carbon nanotube" Physica E, volume 70(c), 2015, pages 90-100.
[14] Li C, Chou T-W. A structural mechanics approach for the analysis of carbon nanotubes. Int J Solids Struct 2003; 40:2487–99.
[15] Tserpes KI, Papanikos P. Finite element modeling of single-walled carbon nanotubes. Compos Part B Eng 2005; 36:468–77.
[16] Xiao JR, Gama BA, Gillespie Jr JW. An analytical molecular structural mechanics model for the mechanical properties of carbon nanotubes. Int J Solids Struct 2005; 42:3075–92.
[17] Sun X, Zhao W. Prediction of stiffness and strength of single-walled carbon canotubes by molecular-mechanics based finite element approach. Mater Sci Eng 2005; 390:366–71.
[18] Li, C. and Chou, T.-W. (2003), A structural mechanics approach for the analysis of carbon nanotubes, Int. J. Solids Struct., Vol. 40, pp. 2487-99.
[19] Li, C. and Chou, T.-W. (2003), Single-walled carbon nanotubes as ultrahigh frequency nano mechanical resonators, Physical Review B – Condensed Matter and Materials Physics, Vol. 68, pp. 734051-3.
[20] G.I Giannopoulos P.A. kakavas and N.K.Anifantis,(2008), Evaluation of the effective mechanical properties of single walled carbon nanotubes using a spring based finite element approach , Computational Meterial science, Vol. 41, p. 561-569.
[21] Tserpes KI, Papanikos P, Tsirkas S. A progressive fracture model for carbon nanotubes. Composites: Part B 37 (2006) 662–669.
[22] Yu MF, Lourie O, Dyer MJ, Moloni K, Kelly TF, Ruoff RS. Strength and breaking mechanism of multiwalled carbon nanotubes under tensile load. Science 2000; 287:637.