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Full Length Research Paper

Limited component examination of crisscross and easy chair sort single wall carbon nanotube

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A carbon nanotube (CNT) possesses superior mechanical, electrical and optical properties. The stiffness and flexibility is much higher than those of conventional fibers. Various investigators have carried out various experiments as well as theoretical analysis which show that the carbon nanotubes possess superior mechanical properties. The model development in this work is based on the assumption that carbon nanotubes, when subjected to loading, behave like space-frame structures. The bonds between carbon atoms are considered as connecting load-carrying members, while the carbon atoms as joints of the members. To create the finite element (FE) models, nodes are placed at the locations of carbon atoms and the bonds between them are modeled using ANSYS spring element. The present work predicts the Young's modulus variation with respect to different wall thickness. The compiled result shows the Young's modulus variation as well as the comparison of zigzag and armchair type of carbon nanotube due to different loading conditions. The results would act as a useful tool for developing new nano composites.

Key words: Finite element analysis, carbon nanotube (CNT), Young's modulus.

INTRODUCTION

The carbon nanotube was invented by Iijima in early 1990s and it has attracted the attention of researchers. The tubes are hollow cylinders with diameters ranging from 1 to 50 nm and having a length in the range of micrometers. They only contain carbon atoms and can be thought of a seamless cylinder rolled from a graphite sheet. The carbon nanotubes (CNT) are produced by various techniques such as arc discharge, laser ablation and chemical vapor decomposition. Extensive experiments using various advanced measurement tools have been carried out to identify the mechanical properties and the behaviors of CNT including the Young's modulus, shear modulus, buckling behavior and vibration responses. Treacy et al. (1996) assessed the Young's modulus of multi walled carbon nanotube cantilevered under thermal vibration based on the measured free end amplitude in a transmission electron microscopy (TEM). For finding the values of the Young's modulus of carbon nanotubes, various methods has been implemented by various researchers. A cantilevered beam model was used by Wong et al. (1997) in which multi walled carbon nanotube was bent using an atomic force microscope tip. By fitting the measured static response to the analytical solution for a cantilevered beam, a Young's modulus of 1.28 ± 0.59 TPa was obtained. The bar model has been used in experiment by Lourie and Wanger (1998), in which the compressive response was measured by using micro Raman spectroscopy. They reported Young's modulus of 2.8 to 3.6 TPa for singled walled carbon nanotubes (SWCNT) and 1.7 to 2.4 TPa for multi walled carbon nanotubes (MWCNT). An average Young's modulus value of 0.90 TPa to 1.7 TPa from measured amplitudes of 27 SWCNT was reported by Krishnan et al. (1998) using analysis of thermal vibration. Poncharal et al. (1999) measured the resonance frequency of MWCNTs by driving the resonance with a counter electrode and RF excitation. They obtained the Young's modulus of approximately 1

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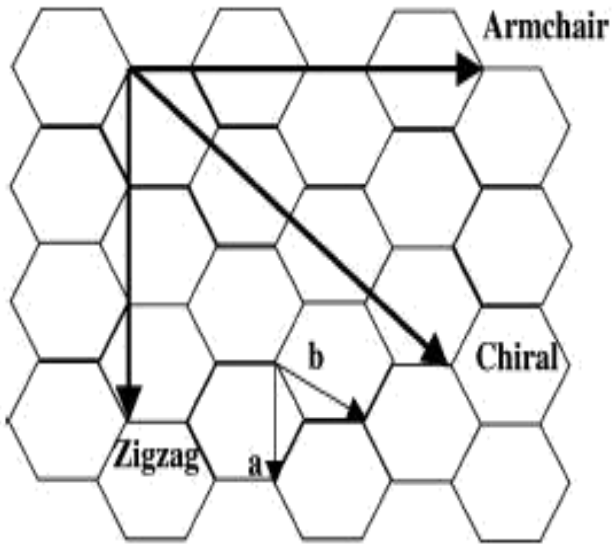

Figure 1. Shows the roll up vectors as a linear combinations of base vectors.

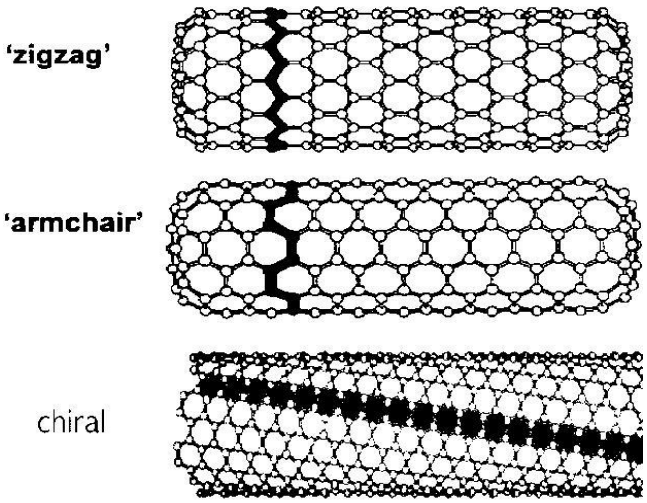

Figure 2. Shows the types of CNT.

TPa with radius smaller than 12 nm; when the resonance response was fit by the assumption of a homogeneous resonating beam for a larger diameter MWCNT, a sharp drop in Young's modulus was fit. The Young's modulus obtained ranges from 320 to 1470 GPa for single walled carbon nanotube (SWCNT) (Yu et al., 2000a), and 270 to 950 GPa for multi walled carbon nanotube (MWCNT) (Yu et al., 2000b). The simply supported beam model was used and predicted the Young's modulus of 1 TPa for MWCNT.

The finite element method has been developed recently and has been adopted to characterize the mechanical response of SWCNT in a number of works. A continuum finite element approach for modeling the structure and the deformation of single and multi wall nanotubes was published by Pantato et al. (2004). Individual tubes were modeled using the shell elements where a specific pairing of elastic properties and mechanical thickness of the tube wall was identified to enable successful modeling with the shell theory. A Young's modulus around 4.84 TPa was computed for the wall thickness 0.075 nm in his work. Tserpes and Papanikos (2005) proposed a three dimension finite element model for armchair, zigzag and chiral type of SWCNT which was based on the assumption that SWCNTs behave like a beamed structures under loading conditions. They concluded that Young's modulus varies from 0.952 to 1.066 TPa and the shear modulus from 0.242 to 0.504 TPa for a wall thickness of 0.34 nm. Finally, the elastic properties that is, the Young's modulus and the shear modulus of SWCNT were computed via finite element method by To (2006). To's method (To, 2006) introduced the Poisson effect in the estimation of the Young's modulus and the shear modulus of SWCNT. The values obtained were around 1.03 and 0.475 TPa for Young's modulus and shear modulus respectively. The wall thickness assumed was 0.34 nm. Li and Chou (2003) gave us a theoretical approach to determine the elastic properties of carbon nanotube.

In this paper, a three-dimensional (3D) finite element model for zigzag single walled carbon nanotube is proposed in order to compute the mechanical response of single wall carbon nanotube. The inter atomic interactions are modeled using the elastic spring element. The element used is ANSYS 11 spring element.

ATOMIC STRUCTURE OF CARBON NANOTUBES

The following types of carbon nanotubes are:

1. Singled walled carbon nanotubes (SWCNT).
2. Multi walled carbon nanotubes (MWCNT).

A wide approach to the identification of SWCNT is by the reference of rolling up the graphene sheet. The key geometric parameter associated with this process is the roll up vector "r", which can be expressed as the linear combination of the lattice basis (a and b) (Figure 1).

The following relation holds good:

$$r = na + mb \quad (1)$$

Where, n = 0 for "zigzag", n = m for "armchair", Other for "chiral" (Figure 2).

The MWCNT are concentric SWCNT. The effect of the curvature on the interlayer distance 0.342 to 0.36 nm and is a function of the curvature and the number of layers. The C–C bonds have a length of 0.1421 nm, which is shorter than the bonds in diamond, indicating that the

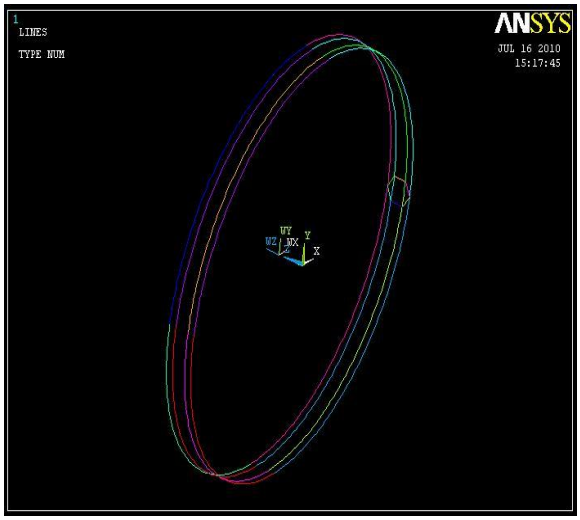

Figure 3. Base circle
Figure 3. Base circle.

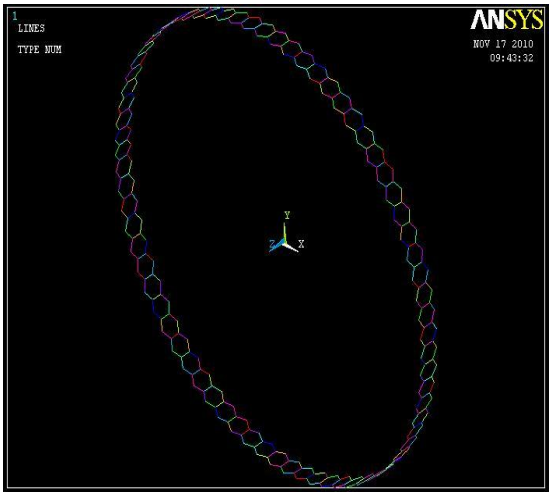

Figure 4. Hexagon linkages.
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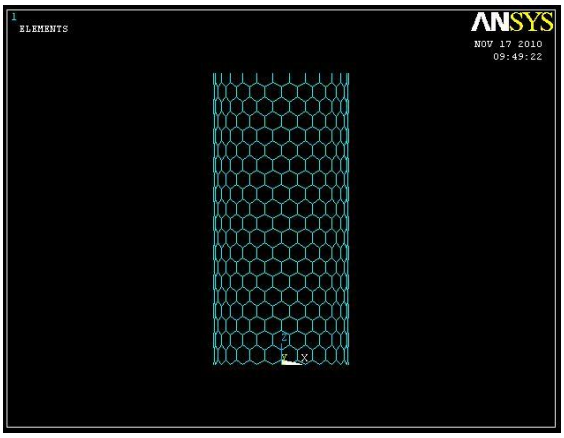

Figure 5. Meshed structure (zigzag).

material is stronger than diamond.

FINITE ELEMENT MODELING

It has been stated that carbon nanotubes are bonded together with covalent bonds which forms the hexagonal lattice as show in Figure 4. These bonds are characterized by bond length and a bond angle. The displacement of individual atoms under the axial force is constrained by the bonds. Therefore, the total deformation of the nanotube is the result of the interactions between the bonds. The bonds are considered as connecting load carrying elements and the atoms as joints of the connecting elements. The CNTs are simulated as space frame structures. The single walled carbon nanotube is modeled using the ANSYS 11 software. The wall thickness of the tube is considered to be equal to that of cross sectional diameter of the element. The element chosen is COMBIN 40 which is a combination of spring-slider-damper element. The damping coefficient and the limiting sliding is considered in order to provide an effect of the weak Vander Waals forces in CNTs. In this work the carbon atoms are considered as nodes and the bonds are considered as the elements. The model is meshed and the boundary conditions are applied. The tube is fixed at one end with all degrees of motion arrested at one end and an axial load is applied on the other end as shown in the Figures 9 and 10.

Figure 4. Hexagon linkages.

Proposed methodologies

Design procedure of single wall zigzag carbon nanotube:

a. Define analysis type.
b. Define the element type. Element chosen is COMBIN 40.
c. Define real constants of the element.
d. Define the material properties.
e. The single wall carbon nanotube is modeled using lines and keypoints as shown in Figure 3.
f. Finite element meshing is done for zigzag and arm chair type as shown in Figure 5 and 6.
g. The boundary conditions are applied. All degrees of freedom of each node is arrested on one end of the structure while an axial force is applied on on each node the other end as shown in Figure 7 and 8.
h. Solve the problem.
i. Post processing. Nodal solution is obtained and the Z-component of displacement is obtained.
j. Young's modulus is calculated.

Elastic moduli of the elements and spring stiffness

To calculate the elastic moduli of the elements, a linkage between molecular and continuum mechanics is used which was given by Li and Chou (2003). From the

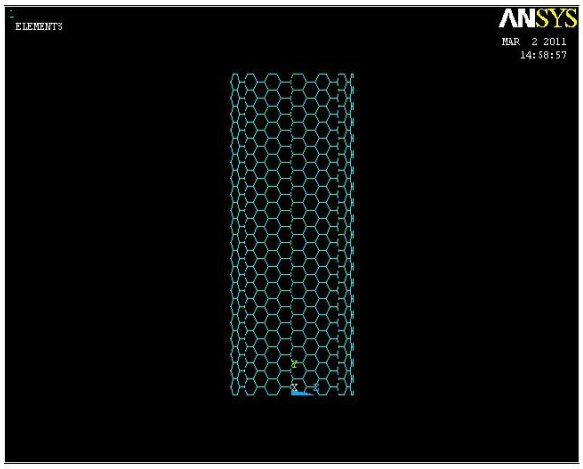

Figure 6. Meshed structure (armchair).

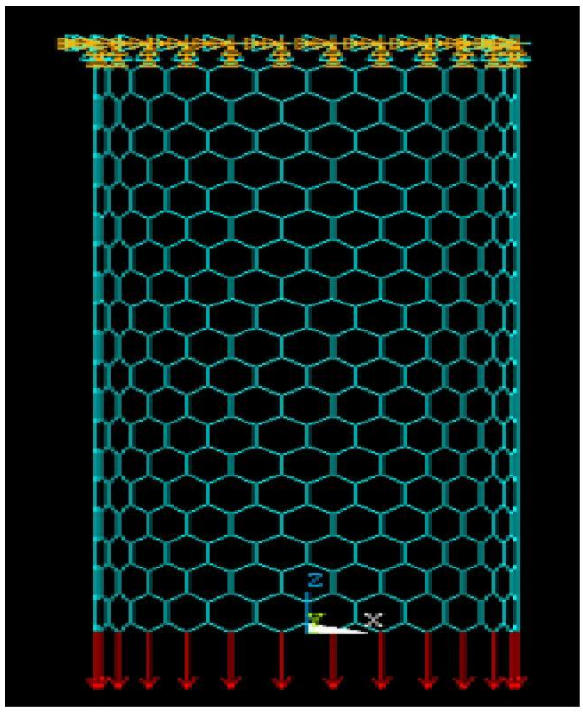

Figure 7. Boundary conditions (zigzag).

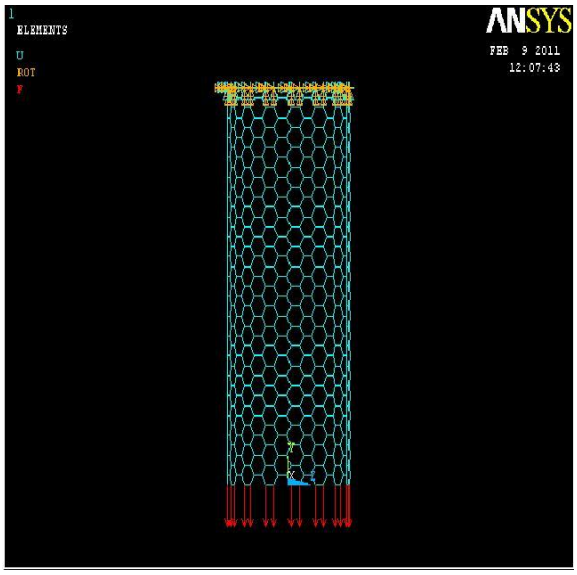

Figure 8. Boundary conditions (armchair).

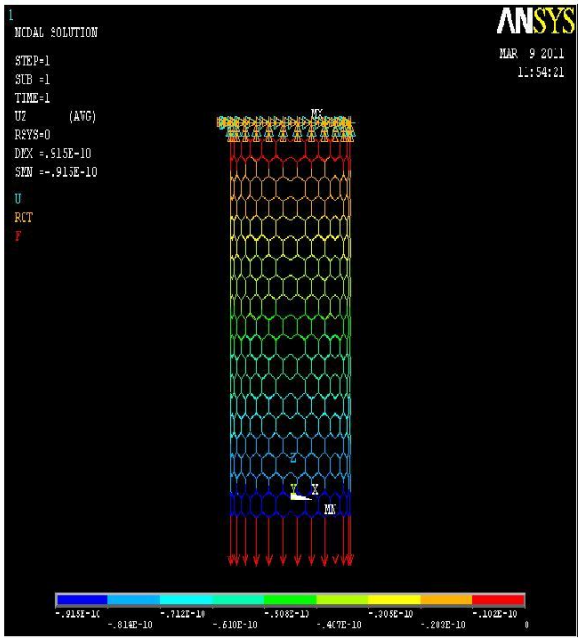

Figure 9. Zigzag simulation in ANSYS.

viewpoint of molecular mechanics, CNTs may be regarded as large molecules consisting of carbon atoms. In order to determine the elastic modulii of the elements, relation between the section stiffness parameters in structural mechanics and the force field constants in the molecular mechanics is to be calculated. For simplicity the cross sectional area of the bonds is assumed to be circular. The elastic modulus ,Y, can be determined by equating the energies due to the interatomic interactions and the energies due to deformation of the structural elements of the space frame. According to the classical structural mechanics, the strain energy of a spring element under axial force N is given by

$$Strain\ energy\ of\ a\ spring = \frac{1}{2} x\ force\ x\ deflection \quad (2)$$

Comparing the molecular mechanics and the classical mechanics, the expressions for the force constants k_Y and

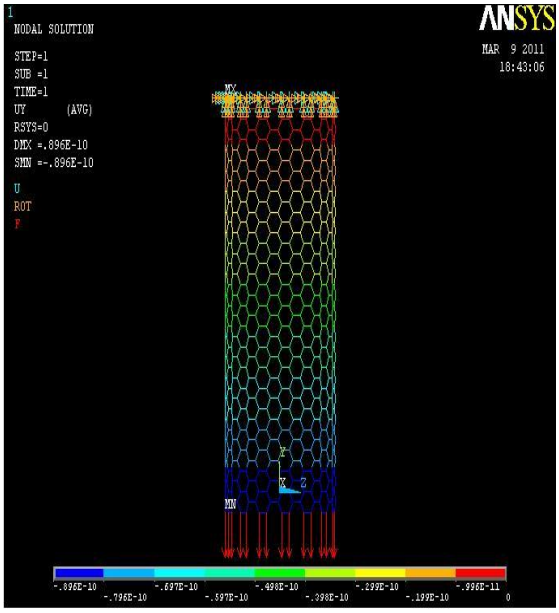

Figure 10. Armchair simulation in ANSYS.

k_T are given as

$$k_r = \frac{EA}{L} \quad (3)$$

$$k_\tau = \frac{EI}{L} \quad (4)$$

The values for $k_Y = 6.52 \times 10^{-7}$ N/nm and $k_T = 2.78 \times 10^{-10}$ N nm rad^{-2} (Tserpes and Papanikos, 2005).

Equations (3) and (4) are the basis for the application of structural mechanics to the analysis of CNTs and carbon related nano structures. Therefore it gives,

$$E = \frac{k_r^2 L}{4\pi k_\tau} \quad (5)$$

The stiffness of the spring, k element is given by

$$k = \frac{(E_{element} \; x \; A)}{L} \quad (6)$$

Where A is the circular cross sectional area, L is the length of each element and E is the elastic modulus of the element.

RESULTS AND DISCUSSION

Effect of wall thickness on Young's modulus

An axial force is applied at one end of the carbon nanotube. The Young's modulus of the tube is calculated corresponding to different wall thickness. Keeping the tube length and the tube diameter to be constant Young's modulus for various wall thicknesses has been calculated as shown in the Table 1. The formula used for calculation of Young's modulus(Y) is

$$Y = \frac{F/A}{\partial L/L} \quad (7)$$

Where F is the axial force applied, A is the cross sectional area, ∂L is the change in length and L is the length of the tube.

The Young's modulus corresponding to different wall thickness are enlisted in Table 2. The values are then plotted graphically as shown in Figure 11. Thus, from the graph it was found that the Young's modulus of a single walled carbon nanotube is inversely proportional to the wall thickness. The relation between the Young's modulus and the wall thickness was also given by Tserpes and Papanikos (2005). The relation given by the present model agrees very well with the relation as given by Tserpes and Papanikos (2005). The difference in the Young's modulus corresponding to the different wall thickness is due to the difference in tube diameter and the element used in the literature. The present work would be helpful in knowing the behaviour of carbon nanotubes of different wall thickness and various nano composites.

Various other investigators have also proposed the Young's modulus as shown in Table 2. The present value is quite close to the values as estimated by the eminent investigators.

It has been observed from the Figure 12 that the Young's modulus of zigzag CNT is higher than that of the armchair. The reason may be due to the different orientations of the elements in both the types.

From Figure 13 it has been observed that the arrangement is different in two types of the CNT. In case of the zigzag type force F acts on a single node of the hexagon while in case of the armchair the same force F acts on two nodes of the hexagon. Thus, due to the structural difference the CNTs are subjected to different loading pattern even though the force is constant. Hence, the Young's modulii of the two types of the CNT are different.

Conclusions

A Finite Element (FE) model has been developed for zigzag carbon nanotube. The model is developed assuming that a CNT when subjected to loading behaves like space frame structures. The Finite Element model consists of small number of elements. The advantage in FE methods is that the same method can be used in MWCNT and other CNT based nano composites. The

Table 1. Young's modulus for different wall thickness of a 40 nm length zigzag tube 2 nm diameter.

S/No.	Wall Thickness (nm)	Young's modulus (zigzag) (TPa)	Young's modulus (armchair)(TPa)
1	0.066	3.258590631	2.8603433
2	0.074	3.257849235	2.85912968
3	0.12	3.25740319	2.857239432
4	0.147	3.256383642	2.85704331
5	0.3	3.256250563	2.85636443
6	0.34	3.253628440	2.852462445

Table 2. Young's modulus reported by investigators in literatures.

Investigators	Young's Modulus (TPa)
Present work	3.256684284 (zigzag)(average of 6 reading) 2.8570971(armchair)(average of 6 readings)
Treacy et al. (2006)	1.5 to 5 TPa
Lourie and Wanger (1998)	2.8 – 3.5 TPa
Alzubi et al. (2008)	1.2 to 3.9 TPa
Cai et al. (2009)	0.94 to 5.81 TPa

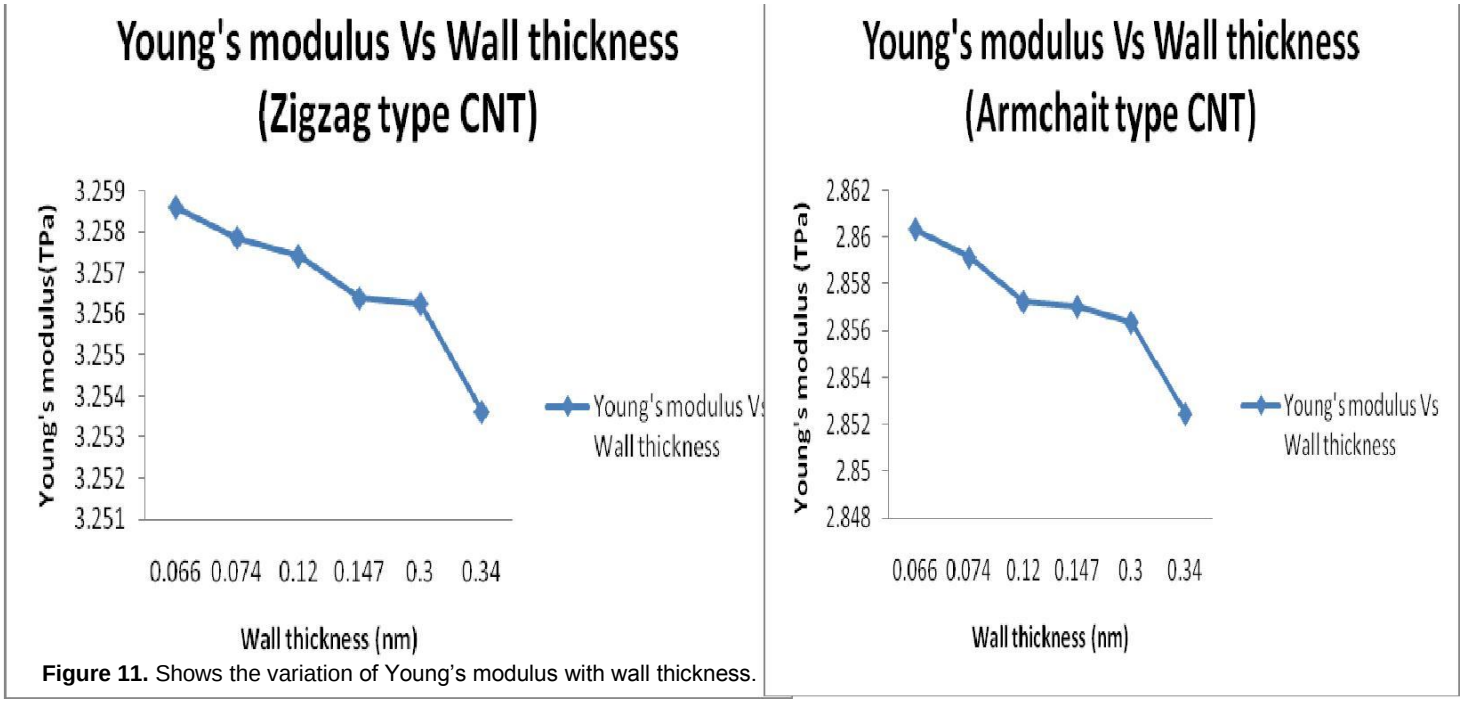

Figure 11. Shows the variation of Young's modulus with wall thickness.

effect of wall thickness on the elastic modulus has been investigated from the FE model. The nonlinear behaviour of the carbon nanotube has also been predicted in the present work. The FE model suggests that Young's modulus is inversely proportional to the wall thickness. The present result may act as a useful tool for studying the mechanical behaviour of CNT and nano composites. It is also being observed that the nonlinear FE model can predict the mechanical response of the single wall carbon nanotube.

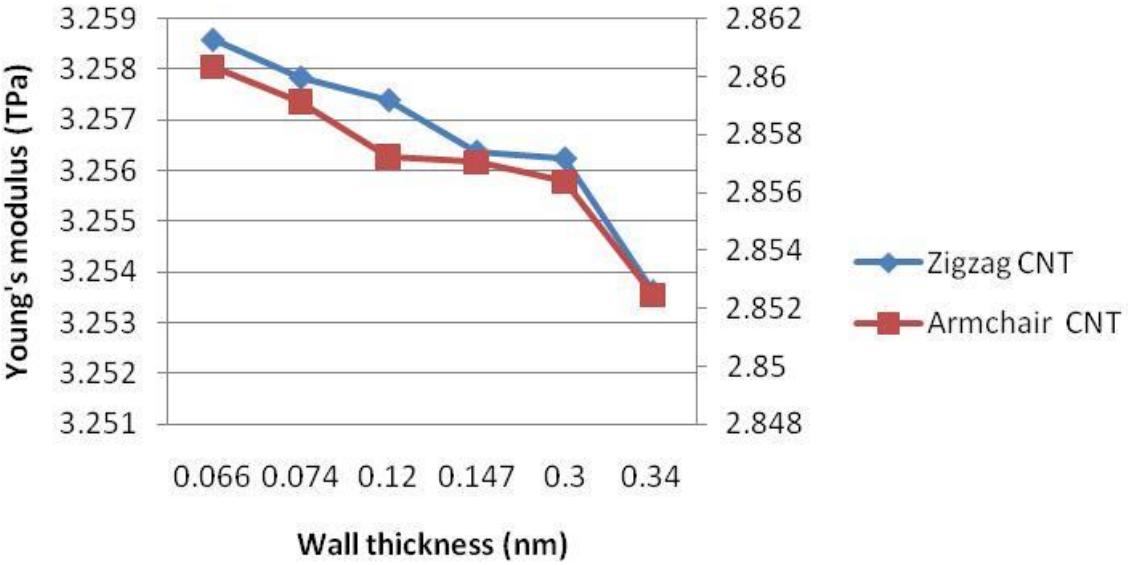

Figure 12. Zigzag Vs Armchair CNT.

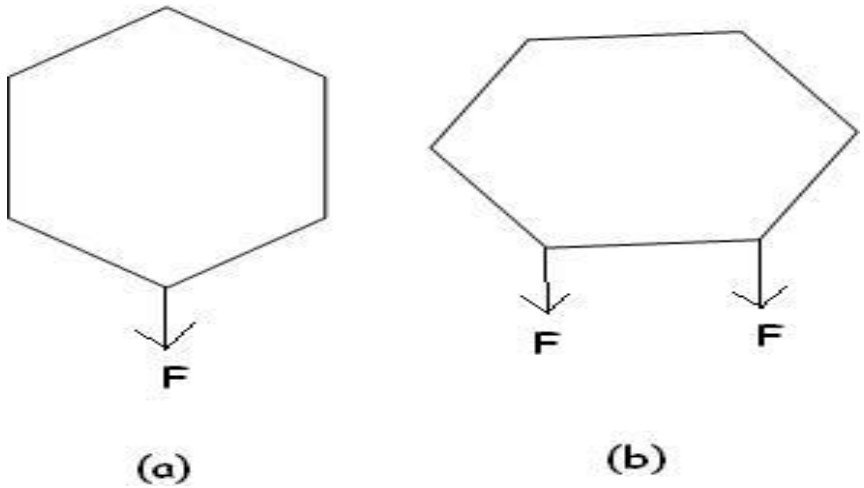

Figure 13. The arrangement of elements in the CNT (a) zigzag (b) armchair.

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