Estmation of Young`S Modulus for Single Walled Carbon Nanotube With Finite Element Method

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Abstract – Much research has been devoted to the study of the mechanical properties of carbon nanptube but still some information is still being disputed. Investigators are trying to find the properties of carbon nanotube because carbon nanotubes possess unique properties for which we can apply in any field. The aim of this paper is, to estimate the Young`s modulus of zigzag and armchair type of carbon nanotube by finite element method. For this we take the assumption that carbon nanotube will act as space frame structure, when load is applied. The bonds between adjacent carbon atoms treated as load carrying members and the carbon atoms as joints of the members. To create finite element models, the carbon atoms are treated as nodes and the bonds between them are modeled using three dimensional beam element with ANSYS software. The Young`s modulus varies with respect to the different wall thickness, lengths and element diameters. The obtained results are matched with the previous results conducted by the various investigators. The results would act as useful tool for developing for new nano composite materials and CNT.

Keywords- carbon nanotube; Zigzag and Armchair; Finite element approach; Beam element; Young`s modulus.

I. INTRODUCTION

Carbon nanotubes (CNT) are members of the fullerene structural family. These are long, thin cylinders of carbon, and discovered in 1991 by Lijima[1]. Due to its unique properties many researchers are conducted different types of experiments on it. The potential use of CNTs as reinforcing materials in nano-composites has originated the need to explore their mechanical properties. CNTs are hollow cylinders in shape. The diameter varies in between 1 to 50 nm and its length is up to few micrometers. For finding the mechanical properties of the CNT such as Young`s modulus, Shear modulus, Buckling, Tensile strength and Vibrations by using advance tools and computer based software. Their name is derived from their long, hollow structure with walls formed by one –atom-thick sheets of carbon, called graphene. CNT possess superior mechanical properties over other conventional fibers as its elasticity is 5 times greater than steel, their tensile strength is maximum 63 GPa and specific strength is 50 times greater than steel. Researchers gave various methods for finding the Young`s modulus of CNT. For examples, experimental investigations conducted by Treacy et al. [2] who used TEM to measure the Young's modulus of MWNTs, reported a mean value of 1.8TPa with a variation from 0.40 to 4.15TPa. Yakobson et al. [3] used the method of molecular dynamics with a wall thickness of 0.066 nm to concluded the young`s modulus as 5.5 TPa. Wong et al. [4] had estimated the elastic modulus as 1.28± 0.59 TPa. By the recently development of the finite element method has been adopted to characterize the mechanical response of SWNT in a number of works. Lu et al. [5], Jin and Yuan et al. [6] are following the method of Molecular Dynamics with thickness of 0.34nm and evaluate the Young`s modulus value of 0.974 TPa and 1.238 TPa .

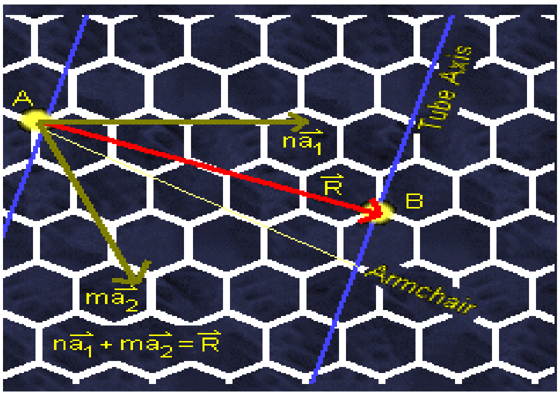

Figure 1.Schematic of nanotube structure

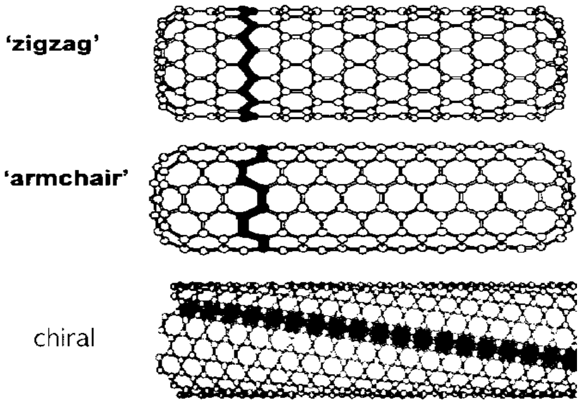

Figure 2.Types of CNT

Yu et al. [7] have demonstrated the use of atomic force microscopy (AFM) to measure the mechanical properties of single walled carbon nanotubes (MWCNTs). They have suggested the tensile strength and modulus range from 11 to 63GPa and 0.27 to 0.95TPa, respectively. T serpes and Papanikos [8] developed a three dimension finite model for armchair, zigzag and chiral type of SWCNT, that is based on the assumption of SWCNT behave like a beamed structures when load is applied. They given the values of Young`s modulus and Shear modulus in the range of 0.952 to 1.066 TPa and 0.242 to 0.504 TPa for a wall thickness of 0.34 nm. To`s [9] estimated the Young`s modulus and Shear modulus of SWCNT by finite element method with the effect of Poisson and wall thickness assumed as 0.34 nm, the values are 1.03and 0.475TPa.

The main objective of this paper is to compute the elastic property (Young`s modulus) of a three dimensional finite element model of Zigzag and Armchair type single walled carbon nanotube(SWCNT).For this we choose a beam element as the joint between the two adjacent carbon atoms. ANSYS 11 version 3D beam4 element is used.

II. STRUCTURE OF CARBON NANOTUBE (CNT)

Carbon nanotubes (CNTs) are allotropes of carbon with a cylindrical nanostructure. CNTs are the strongest and stiffest materials yet discovered in terms of tensile strength and elastic modulus. CNT`s have remarkable electronic, mechanical and chemical properties.

Carbon nanotubes are two types:

a) Single walled carbon nanotube (SWNTs)
b) Multi walled carbon nanotube (MWNTs)

There are several ways to view a SWCNT. The most widely used is by reference to rolling up grapheme sheet to form a hollow cylinder. SWNTs forms different types, which can be described by the chiral vector equation (see figure 1.)

$$R = n a_1 + m a_2 \qquad (1)$$

Where a_1 , a_2 = vectors
n, m = integers of the vector equation.

SWCNTs are classified into three different types. (1) Zigzag (n,0) (2) Armchair (n, n) (3) Chiral (n, m) (see figure 2 & 4). The diameter of an ideal nanotube can be calculated from its (n, m) indices as follows

$$\text{Tube diameter} = \frac{\sqrt{3}}{\pi} L \,[\sqrt{(n^2 + nm + m^2)}] \qquad (2)$$

L= C-C bond length (Fig. 5)

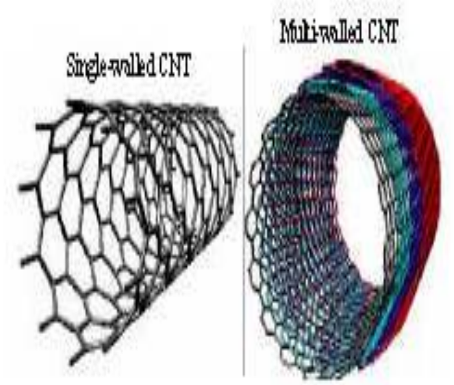

Fig 3: SWNT and MWNT types

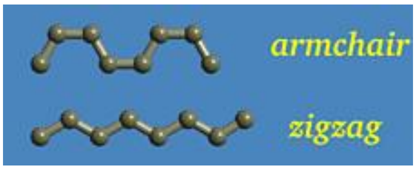

Fig 4.Armchair and Zigzag structure

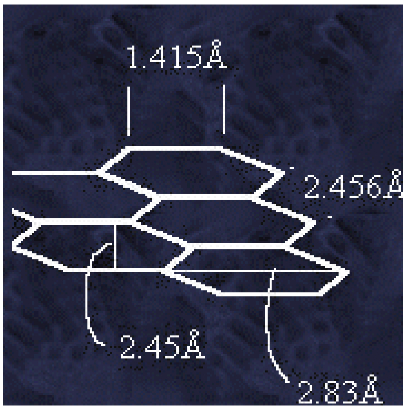

Figure 5.Carbon bond length and Atom spacings of the lattice structure [10].

The bond length is less when compared with the bond length in diamond. That indicates this material is stronger than diamond. The MWCNT are concentric SWCNT that why they will have cylinders within the cylinders (Fig.3).

III. DEFINITION OF ELASTIC MODULUS AND DIAMETER OF ELEMENT:

The three dimensional zigzag and armchair type carbon nanotube models are drawn with the use of PRO-Engineer (version 4.0) software. Then these models are imported into ANSYS software through IGES file. The imported 3D models are recreated using the ANSYS commercial FE model. To create the FE models, nodes are placed at the locations of carbon atoms and the covalent bonds between them are modeled using three-dimensional elastic BEAM4 ANSYS elements.

A BEAM4 ANSYS element is a uniaxial element with have the capabilities of tension, compression, bending and torsion. The element has six degree of freedom at each node: translations in the nodal x, y, and z directions and rotation about the nodal x, y, and z axes. The element is defined by two or three nodes, the cross-sectional area, two area moments of inertia (IZZ and IYY) and material properties. The cross sections of the beam elements are assumed to be uniform and circular, and the necessary input data of the BEAM4 elements are the Young`s modulus E, the Poisson's ratio m and the diameter of the circular cross section element is d_b.

To calculate the Young`s modulus of the elements, a linkage between molecular and continuum mechanics is used which was proposed by the Li and Chou [11]. That is, a linkage between the force field constants in molecular mechanics and the element stiffness parameters in structural mechanics through the energy equivalence concept. From the viewpoint of molecular mechanics, CNTs may be regarded as molecules consisting of carbon atoms. The elastic modulus (E) can be determined by equating the energies due to the inter-atomic interactions and the energies due to deformation of the structural elements of the space frame.

Molecular mechanics = Structural mechanics

$$K_r = \frac{EA}{L}, \quad K_\Theta = \frac{EI}{L}, \quad K_\tau = \frac{GJ}{L} \qquad (3)$$

K_r, K_Θ, K_τ are the force constants, there values are $6.53 \times 10^{-7}\ N/nm$, $8.79 \times 10^{-10}\ N\ nm/rad^2$, $2.78 \times 10^{-10}\ N\ nm/rad^2$ [8] and $\frac{EA}{L}, \frac{EI}{L}, \frac{GJ}{L}$ are the element stiffness. By using above equation the diameter of tube and elastic modulus of the elements are

$$d_b = 4\sqrt{\frac{K_\Theta}{K_r}} \qquad (4)$$

$$E = \frac{L{K_r}^2}{4\pi K_\Theta} \qquad (5)$$

It has been stated that CNTs are bonded together with covalent bonds which forms hexagonal. These bonds are characterized by the bond length and a bond angle. By using the dimensions of carbon nanotube(diameter of tube, bond length between the c-c atoms, and bond angle), hexagonal are drawn with PRO-E software (version 4.0) commands. That is SWCNTs (both zigzag and armchair type) are modeled by using both PRO-E and ANSYS 11 software.

For modeling of SWCNT in PRO-E, we follow this way:

a. Select the new file and choose the Part modeling.
b. Select the extrude command.

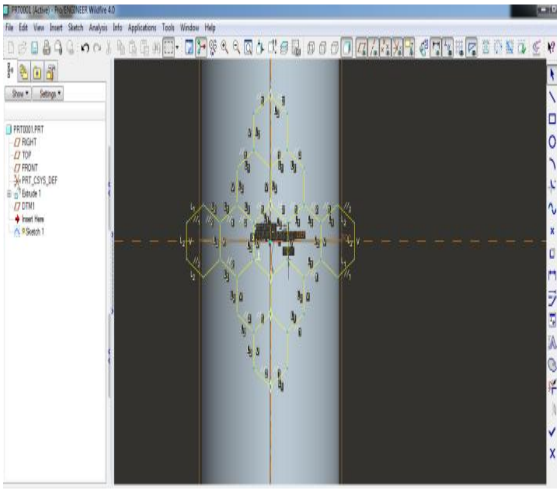

Figure 6: Drawing of carbon nanotube with PRO-E software.

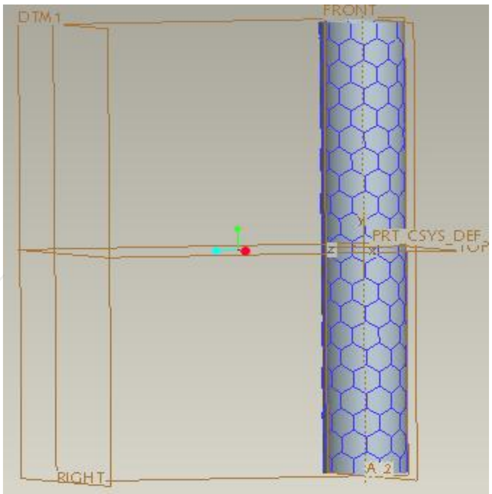

Fig 7: Drawing of carbon nanotube with PRO-E software.

c. Draw the hollow cylinder with required diameter and length. (Following the dimensions of CNT). (Fig. 6)
d. Take the datum plane and hexagonal are drawn on it, (Following the dimensions of bond length and bond angle) and do some operations. (Fig. 7).

The PRO-E based modeled of CNT is imported into the ANSYS software through IGES files option. The bonds are considered as load carrying elements and atoms as joints of the carrying elements. The carbon nanotubes are simulated as space frame structures. In ANSYS software, we choose BEAM4 as element type. In this present work, atoms of carbon are considered as nodes and bonds between the atoms are taken as elements.

IV. PROCEDURE FOR DESIGN OF SINGLE WALLED CARBON NANOTUBE

The Design procedure in ANSYS can be broadly classified into

Pre processing
Processing
Post processing

Pre-Processing:

Pre processing consists of model generation and discreatization into finite elements.

The following operations are done:

a. To define the analysis type. (Structural analysis)
b. To define the element type. (BEAM4 element)
c. To define the real constants and material properties of the element.
d. The imported version of single walled carbon nanotube from the PRO-E software is remodeled in the ANSYS.

Finite element meshing is done to both the Zigzag and Armchair type SWCNT by using meshing command. (Fig. 8)

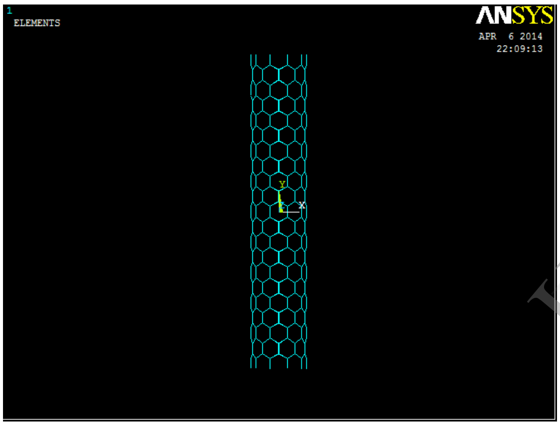

Fig 8.Model of Zigzag type with meshing

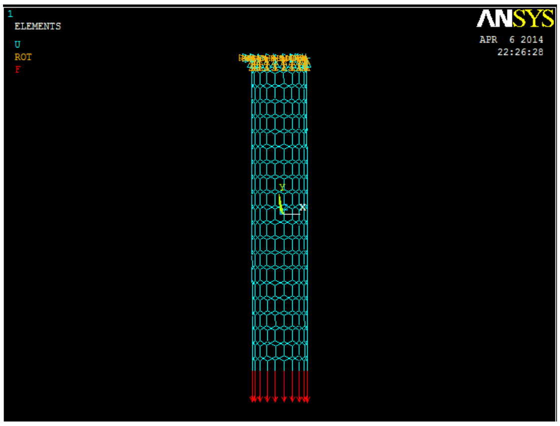

Fig 9.Boundary condition on Zigzag type

Processing (solution):

After pre processing phase, the model is in second phase, i.e. processing phase in which the analysis will get the solution. Boundary conditions are applied and solution procedures are performed. Structural static analysis is used to determine the displacements, stresses, strains and forces that occur in the continuum as a result of applied loads.

The following operations are done:

a. The boundary conditions are applied such that all degree of freedom of each node is arrested on one end of the structure while other end an axial force is applied on each node. (fig 9)

b. By using Current Load Step (LS), solve the problem.

Post Processing:

The third (or) final phase is Post Processing. In this phase, the results of the problem are displayed in the form of charts, tables and graphs.

The following ways are used for results obtained:

a. Display the boundary conditions.
b. Nodal solution is obtained and the Y- displacement component is obtained.
c. By using formula axial Young`s modulus is calculated.

V. RESULTS AND DISCUSSION:

The bonds are restricted the displacement of individual atoms in the CNT under axial force. Therefore, the total deformation of the carbon nanotube is the result of the interaction between the atoms. Finite element analysis results are used to compute the axial Young’s modulus of carbon nanotube.

The formula used to calculated the axial Young`s modulus (Y) is

$$Y = \frac{F/A}{dl/L} \qquad (6)$$

Where F = axial force applied
A = cross sectional area
dl = change in length
L = length of the tube.

The objective of the paper is to calculate the axial Young`s modulus value when

1. Various wall thicknesses.
2. Change the tube length.

3. Change the diameter of the element (BEAM4 element).

1. Effect of wall thickness of the CNT on Young`s modulus

The Young`s modulus value is calculated with respect to the different wall thickness, when an axial force is applied on each node of the CNT on one end and the another end is fixed (Fig. 10&11). Consider the applied force and the length of the tube as constants. Diameter of the tube is varies. By using the Y-component of displacement value (dl) from ANSYS, we calculate the young`s modulus value with the formula (From equation 6).

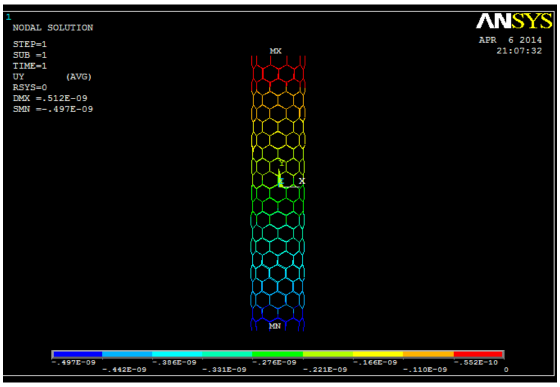

Fig 10. Y-component of displacement value of Zigzag type in ANSYS (for tube diameter 0.78025 nm)

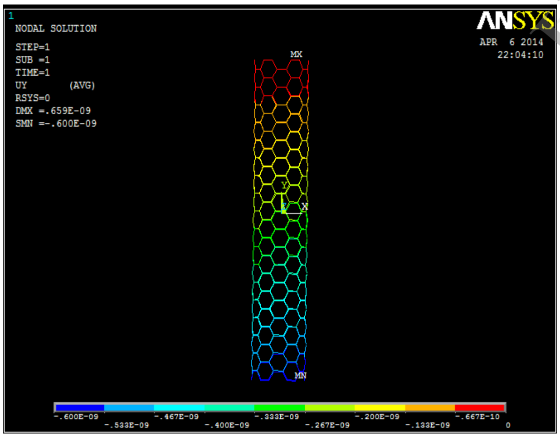

Fig 11. Y-component of displacement value of Armchair type in ANSYS (for tube diameter 0.81074 nm)

The young`s modulus value with respect to the different wall thickness are noticed in the tables. The tables give the information of Young`s modulus value various with respect to the different wall thickness. (from tables 1&2)

The obtained Young`s modulus value for different wall thicknesses are presented in the table (1&2), graphs are drawn based on these values. From graph (Fig. 16 & 17) we concluded that the (a) Young`s modulus is inversely proportional to the wall thickness of CNT (both Zigzag and Armchair) i.e. as when the wall thickness is reduces the Young`s modulus value is more.

(b) Young`s modulus is directly proportional to tube diameter of CNT (both Zigzag and Armchair) i.e. when tube diameter increases the Young`s modulus value also increases.

2. Effect of tube length of the CNT on Young`s modulus

The Young`s modulus value is calculated with respect to the different tube lengths, when an axial force is applied on each node of the CNT on one end and the another end is fixed (Fig. 12 & 13). Consider the applied force, thickness of the wall (0.34 nm) and diameter of the tube are taken as constants. By using the Y-component of displacement value (dl) from ANSYS, we calculate the young`s modulus value with the formula (From equation 6).

Figures 12 (a, b, c) and 13 (a, b, c) are Y-component of displacement values in ANSYS for different tube lengths.

The axial Young`s modulus value with respect to the different tube lengths are noticed in the table. The table give the information of Young`s modulus value varies with respect to the different tube lengths.

Zigzag type tube lengths:

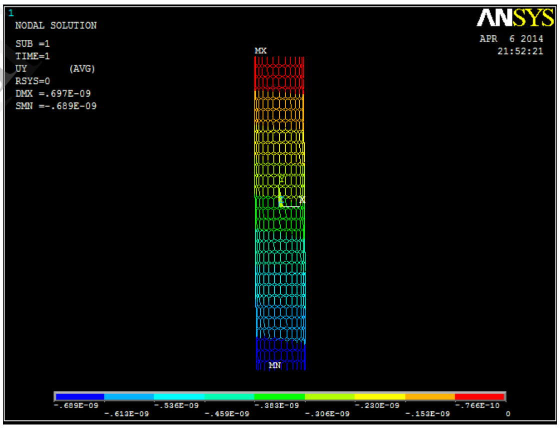

Fig 12(a): Y-component of displacement value of Zigzag type in ANSYS (for tube length 6.085 nm)

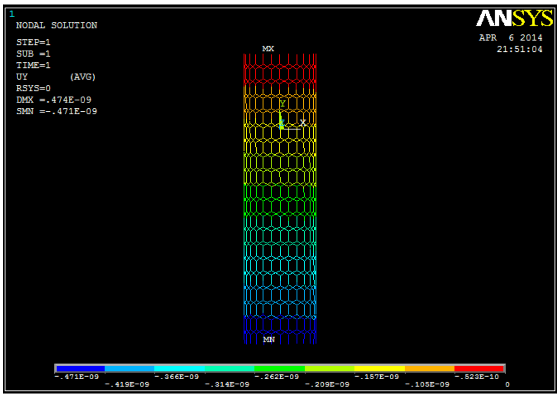

Fig 12(b): Y-component of displacement value of Zigzag type in ANSYS (for tube length 4.176 nm)

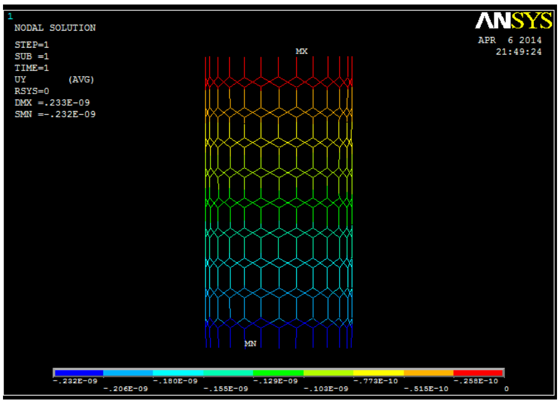

Fig 12(c): Y-component of displacement value of Zigzag type in ANSYS (for tube length 2.0553 nm)

Armchair type tube lengths:

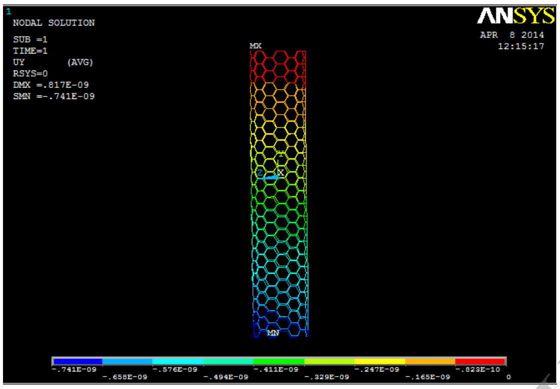

Fig 13(a): Y-component of displacement value of Armchair type in ANSYS (for tube length 5.5149 nm)

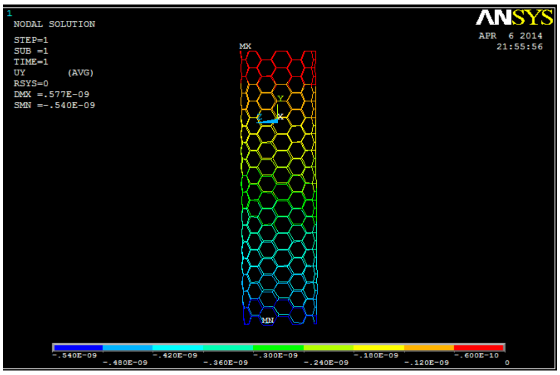

Fig 13(b): Y-component of displacement value of Armchair type in ANSYS (for tube length 4.0445 nm)

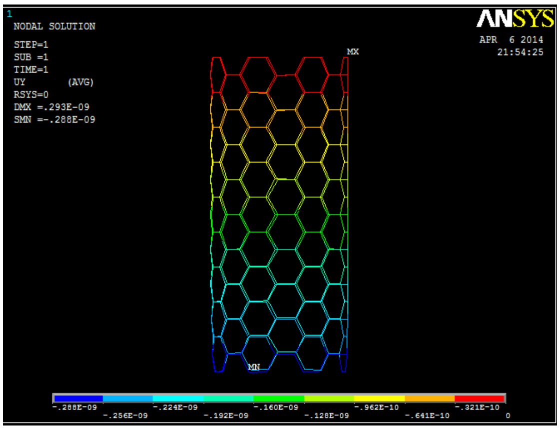

Fig 13(c): Y-component of displacement value of Armchair type in ANSYS (for tube length 2.2058 nm)

3. Effect of element diameter (BEAM4) on Young`s modulus

The axial Young`s modulus value is calculated with respect to the different element diameters, when an axial force is applied on each node of the CNT on one end and the another end is fixed. Consider the applied force, the length of the tube, the diameter of the tube and the thickness of wall (0.34nm) are taken as constants.

In present work, the elements were considered as BEAM4 element. From equation 4, diameter of the element is 0.147 nm (by using the values of K_r , K_θ). Figure 15&16 shows the values for element diameter 0.147 nm. The considered diameters and corresponding Young`s modulus values are shown in the table. By using the equation 6 we calculate the Young`s modulus value .The table given the information of Young`s modulus value varies with respect to the element diameter. (table 5)

From table (5) and graphs (Fig. 20 & 21), shows the variation of Young`s modulus to the element diameter (beam4).As the element diameter varies the young`s modulus value also varies. The Young`s modulus is directly proportional to the Element diameter of CNT. As the element diameter increases the Young`s modulus value increases rapidly (from table 5). For less change in the element diameter, the difference between the young`s modulus values is more. In this case the obtained young`s modulus values of both Zigzag and Armchair type CNTs comes closer to each other. But from the [8], [11] element diameter took as 0.147 nm.

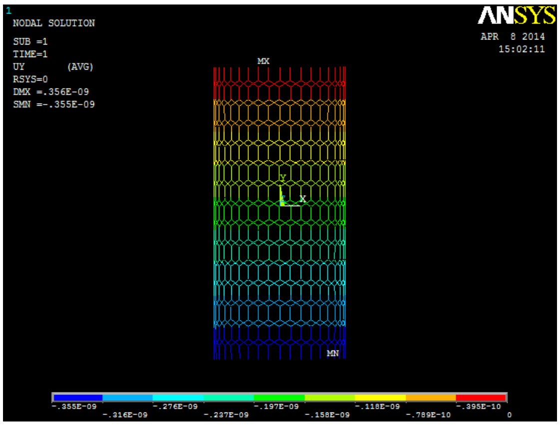

Fig 14: Y-component of displacement value of Zigzag type in ANSYS (for element diameter 0.147 nm)

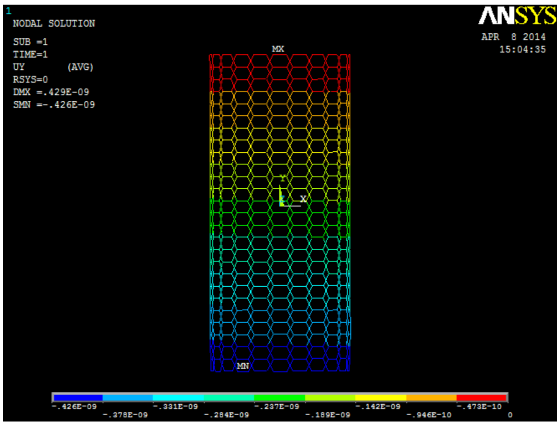

Fig 15: Y-component of displacement value of Armchair type in ANSYS (for element diameter 0.147 nm)

TABLES:

Table 1&2: Young`s modulus of different wall thickness of 4.5 nm length Zigzag and Armchair type tubes.

S/No	Diameter (nm) of Zigzag type	Young`s modulus (TPa) of different Thickness (nm)		
		0.066	*0.12*	*0.34*
1	0.78025	5.285	2.907	1.026
2	0.9364	5.347	2.94	1.038
3	1.0924	5.412	2.976	1.051
4	1.4042	5.523	3.038	1.072

Table 2:

S/No	Diameter (nm) of Armchair type	Young`s modulus (TPa) of different Thickness (nm)		
		0.066	*0.12*	*0.34*
1	0.81074	4.78	2.628	0.928
2	0.9456	5.25	2.888	1.019
3	1.0810	5.34	2.94	1.037
4	1.2162	5.36	2.95	1.040

Table 3&4: Young`s modulus for different lengths of Zigzag and Armchair type CNT with 1 nm tube diameter

S/No	Tube Length (nm) of Zigzag type	Young`s modulus (TPa)
1	6.085	1.0532
2	5.236	1.0596
3	4.600	1.0628
4	4.176	1.0645
5	3.113	1.0656
6	2.055	1.0659

Table 4:

S/No	Tube Length (nm) of Armchair type	Young`s modulus (TPa)
1	5.5149	0.8777
2	4.5346	0.8803
3	4.0445	0.9104
4	3.5544	0.9326
5	2.9410	0.9597
6	2.2058	0.9811

Table 5: Young`s modulus for different element diameters (Beam4) of a 3 nm length Zigzag and Armchair type CNT with 1.5 nm diameter

S/No	**Element Diameter (nm)**	**Young`s modulus (TPa) of Zigzag type**	**Young`s modulus (TPa) of Armchair type**
1	0.1	0.0367	0.0356
2	0.125	0.68	0.6677
3	0.147	1.0568	1.0330
4	0.175	1.6312	1.6070
5	0.2	2.2465	2.2325

GRAPHS:

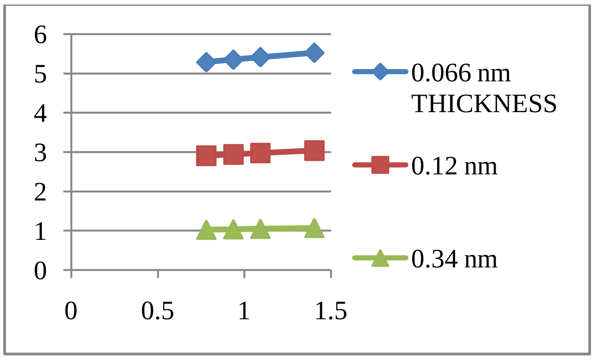

Fig 16: Shows the variation of axial Young`s modulus- Tube diameter (Zigzag type) (values from table 1)

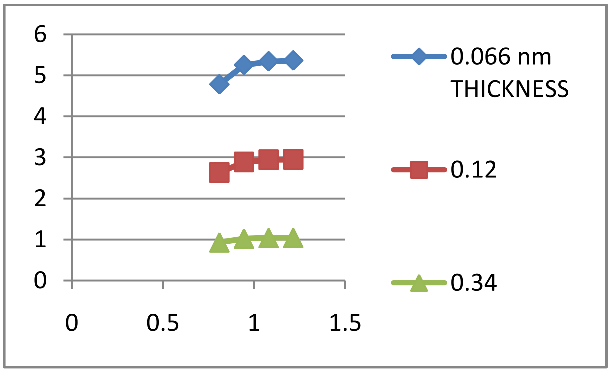

Fig 17: Shows the variation of axial Young`s modulus- Tube diameter (Armchair type) (values from table 2)

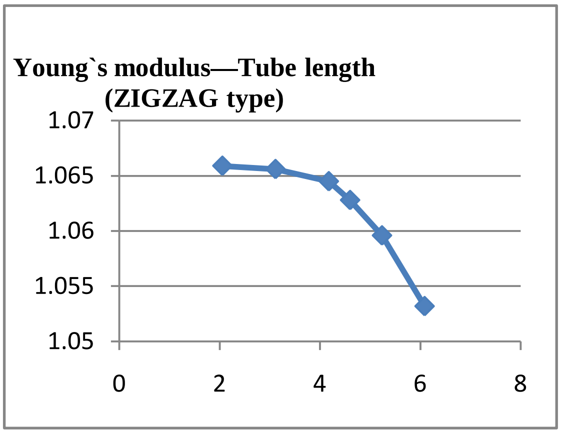

Fig 18: Shows the variation of axial Young`s modulus- Tube length (Zigzag type) (values from table 3)

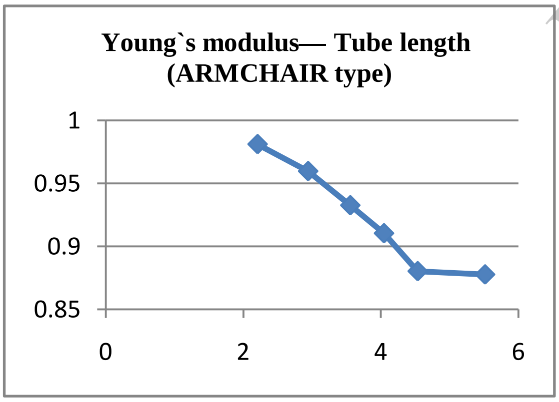

Fig 19: Shows the variation of axial Young`s modulus- Tube length (Armchair type) (values from table 4)

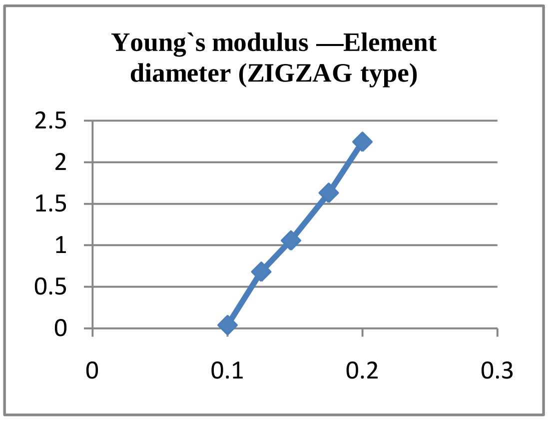

Fig 20: Shows the variation of axial Young`s modulus- Element diameter (Zigzag type) (values from table 5)

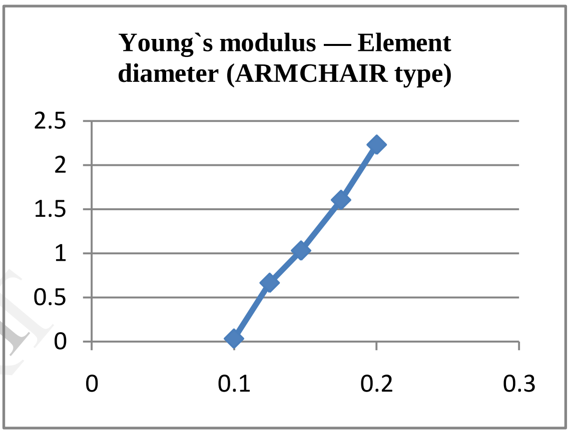

Fig 21: Shows the variation of axial Young`s modulus- Element diameter (Armchair type) (values from table 5)

Various other investigators have also proposed the Young`s modulus as show in the table. The current obtained Young`s modulus values in the above three cases are agreed well to the previous results proposed by the investigators. From the graphs, we observed that the Young`s modulus value of Zigzag type is higher than Armchair type this is due to the chirality, or twist of the tube. From figure 2, we can understand the structure, or configuration of the zigzag and armchair type CNT are different.

Table 6. Young`s modulus reported by investigators in literatures.

	Young`s modulus (TPa)	Thickness(nm)
Yakobson et al. [3]	5.5	0.066
Treacy et al. [2]	1.5 to 5.0	0.34
T serpesa and Panpanikos et al. [8]	1.029	0.34
Li and Chou et al. [11]	1.01	0.34
Cai et al. [12]	0.94 to 5.81	0.34
Georgantzionsa et al. [13]	0.936	0.34
Fan et al. [14]	1.036	0.34
Prabhu et al. [15]	2.85 to 3.26	

VI. CONCLUSION:

A three dimensional finite element model of zigzag and armchair single walled carbon nanotube are developed with the help of PRO-E and ANSYS software. The model is developed, assuming that a CNT when subjected to loading behaves like space frame structures. To create the FE models, nodes are placed at the locations of carbon atoms and the bonds between them are modeled using three-dimensional elastic beam elements. From the Finite element model, how the axial Young`s modulus effected with wall thickness, tube length, and element diameter are computed. Obtained results showed that the wall thickness, tube length are inversely proportional to the Young`s modulus and the element diameter is directly proportional to it. This method can be adopted for MWCNTs with higher number of layers. The obtained results this work may act as useful tool for studying the mechanical behavior of CNT and nano composites.

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