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STUDY THE BEHAVIOR OF ELASTIC MODULUS FOR ZIGZAG AND ARMCHAIR SINGLE WALL CARBON NANOTUBE STRUCTURE WITH FEM

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Abstract: A three-dimensional finite element (FE) model for single-walled carbon nanotubes with armchair and zigzag shapes is proposed in this paper (SWCNTs). Nodes are positioned at the locations of carbon atoms to design the FE models. And three-dimensional elastic beam components are used to model the bonds between them. The effect of the diameter length/diameter ratio on the diameter length/diameter ratio, cross sectional aspect ratio and number of elements on the Young's modulus of SWCNTs has been considered herein. From the conducted experiments it can be observed that, the larger tube diameter can lead to higher Young's modulus for carbon nanotubes. Such that, maximum elastic modulus for the armchair and the zigzag models has be obtained to be 1.0285TPa and 1.0396TPa when the diameters for the armchair and the zigzag models were 2.034nm and 1.957nm respectively. Increasing the length/diameter ratio has led the Young's modulus to be increased for armchair and zigzag models such that its values can reach 1.0451TPa and 1.0191TPa respectively. The cross sectional aspect ratio of SWCNTs showed an inversely proportional effect on the elastic modulus in this work. As a result of rising the cross sectional aspect ratio to be2, the Young's modulus for armchair and zigzag models has decreased to 0.7991TPa and 0.8873TPa, accordingly. The change in geometry has been observed to be a defect and it is in general can decrease the modulus of elasticity. The number of elements in the armchair model considered as prominent factor that increases the young's modulus to be 1.0280TPa when the number of element is 10836. In zigzag model, the number of element has no effect on the elastic modulus since the number of nodes that exposed to the applied load is fixed in this case. The findings showed that the proposed FE model may be useful for studying carbon nanotube mechanical action in the future.

Keywords*; zigzag and armchair, SWCNTs, Young's modulus, Mechanical properties; Finite Element Analysis (FEA).*

1. Introduction

Carbon nanotubes have attracted significant attention since their discovery in 1991by Iijima [1]. Carbon nanotubes have long been regarded as one-of-a-kind valuable nanostructures with a number of remarkable properties that have led to their use in a wide range of fascinating applications. Carbon nanotubes' remarkable properties are largely due to their perfect hexagonal form [2]. Carbon nanotubes (CNTs) have piqued the attention of scientists in recent years due to their peculiar properties. The mechanical, physical, and electrical properties

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of these materials are exceptional. as well as their geometrical characteristics of small diameter and high aspect ratio, CNTs have a broad variety of engineering applications. It has been demonstrated that dispersing a few weight percentages of nanotubes in a matrix greatly improves all of the composite materials' mechanical, thermal, and electrical properties [3]. Scientists would be required to use them as fillers or strengthening agents in composite structures in solid mechanical engineering as a result of these issues. Separately, as well as in smart systems and materials. As a result, To build such structures, the first step is to have a simple and realistic view of carbon nanotube properties, attributes, and attitudes.

A slew of experimental studies have been performed to determine the mechanical properties of CNTs. The mechanical properties of CNTs were determined using transmission electron microscopy (TEM) and atomic force microscopy (AFM) (AFM). There is a lot of variation in these experimental findings due to the difficulty of nano-size characterization. Treacy et al. [4] were the first to calculate Young's modulus in single-walled carbon nanotubes (SWNTs) experimentally in 1996, with approximate values of 0.4–4.15 (average 1.8) TPa. This was accomplished by using TEM to measure thermal vibrations. Wong et al. [5] Individual multi-walled carbon nanotubes (MWNTs) were bent with an AFM tip using a cantilevered beam model. resulting in a lower pressure range of 1.28 0.59 TPa. For SWNTs with diameters ranging from 1.0 to 1.5 nm, Krishnan et al.[6] measured a mean Young's modulus of 1.30.4TPa using TEM. In their experiment, Lourie et al.[7,8] used a bar model and micro-Raman spectroscopy to test the compressive response. They found that SWNT has a Young's modulus of 2.8–3.6 TPa and MWNT has a Young's modulus of 1.7–2.4 TPa. For SWNT [9] and MWNT[10], Direct tensile loading tests were used by Yu et al. The obtained Young's modulus for the SWNT ranged from 0.32 to 1.47 TPa (mean 1.00 TPa), while it ranged from 0.27 to 0.95 TPa for the MWNT. Salvetat et cetera. [11, 12] Individual MWNTs and different-sized SWNTs were studied using a simple-supported beam model in AFM. MWNTs with a Young's modulus of 1 TPa were generated by arc discharge. CNTs made by catalytic decomposition of hydrocarbons, on the other hand, had a modulus that was 1–2 orders of magnitude lower. Using 3-points bending and AFM, Tombler et al. calculated a Young's modulus of 1.2 TPa for SWNT [13].

Although experimental investigations and realistic results are reliable sources in the material design process, There are numerous challenges in carrying out experiments and measurements to evaluate CNT properties at the nanoscale. The small size of nanostructures is the primary source of issues, causing a scatter in experimental outcomes and creating a level of complexity in design and application of smart materials and advanced structures. As a result, computational modeling methods are the best way to test CNT behaviors. In general, two methods for modeling CNTs have been considered. One is molecular simulation, which is thought to be extremely accurate and suitable for molecular systems with a fixed number of atoms. However, in nanostructures, such as large molecules, this approach will be prohibitively expensive in terms of computations and, as a result, It's time to model. Another choice is to use continuum mechanics simulation to model nanostructures. This is thought to be accurate and effective in computations. But from different point of view, The atomic structure and chirality of CNTs are not taken into account by earlier continuum

mechanics simulation techniques. Furthermore, atoms in the CNT system cannot be subjected to point (concentrated) loads, and these models are unable to account for CNT bond faults. For modeling CNTs, atomic structure-based finite element models (FEMs) are recognized as a common method, with benefits such as low accuracy and simplicity.

Low computations and findings that have been confirmed using molecular methods. The molecular structure and properties of single-walled carbon nanotubes (SWCNTs) were linked to continuum mechanics theories using energy equivalence in both systems [14]. Single-walled carbon nanotubes' mechanical response A three-dimensional (3D) finite element model was used to simulate armchair and zigzag single walled carbon nanotubes. The elastic beam factor was used to model the interatomic interactions.

2. Structural design

2.1. Geometrical structure

Carbon nanotubes are in general consisting of carbon atoms which are structured as a layers of graphene forming the shape of the cylinder shown in Fig. 1 .Each carbon atom of a graphene has been designed to be symmetrically bounded to the other three carbon atoms which then forms a hexagonal ring. Carbon nanotubes cylinder has been designed to be open or closed at the ends whereasat an atomic level, graphene shape tends to be as a honeycomb structure. This distinct hexagonal pattern has been replicated on a regular basis, As a consequence, Each carbon atom forms a covalent bond with three neighboring atoms. The covalent bond appears to be a very strong chemical bond that leads to graphene's remarkable mechanical properties, as well as all carbon-related nanostructures as a result.

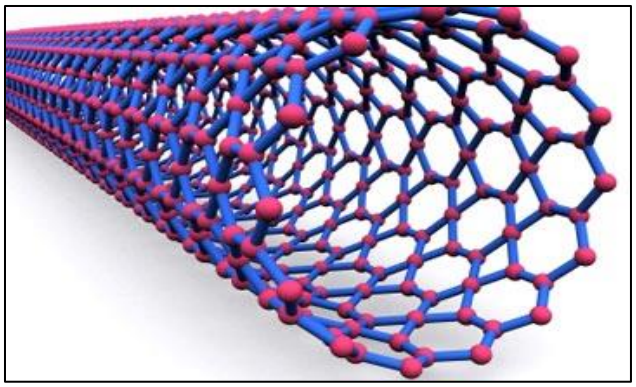


Figure 1. Structure of a carbon nanotube

The atomic structure of CNTs is influenced by tube chirality, The chiral angle expressed by is defined by the chiral or roll-up vector Ch. The chiral vector is written like this: the line connected between two crystallo-graphically equivalently sites O and C in the two-dimensional graphene structure. According to “equation (1)”. [15], the chiral vector can be determined by the two unit vectors, by the two integers m and n, as well as by the two integers a1 and a2 (steps along the unit vectors.

$$C_h = ma_1 \vec{} + na_2 \vec{} \qquad (1)$$

The angle created by the chiral vector Ch and the zigzag direction is known as the chiral angle. Where n = n and m = 0. The zigzagand armchair nanotubes have been designed due tochiral angles of 0 and 30respectively. Figure 2 shows a schematic representation of the two forms of nanotubes [16].

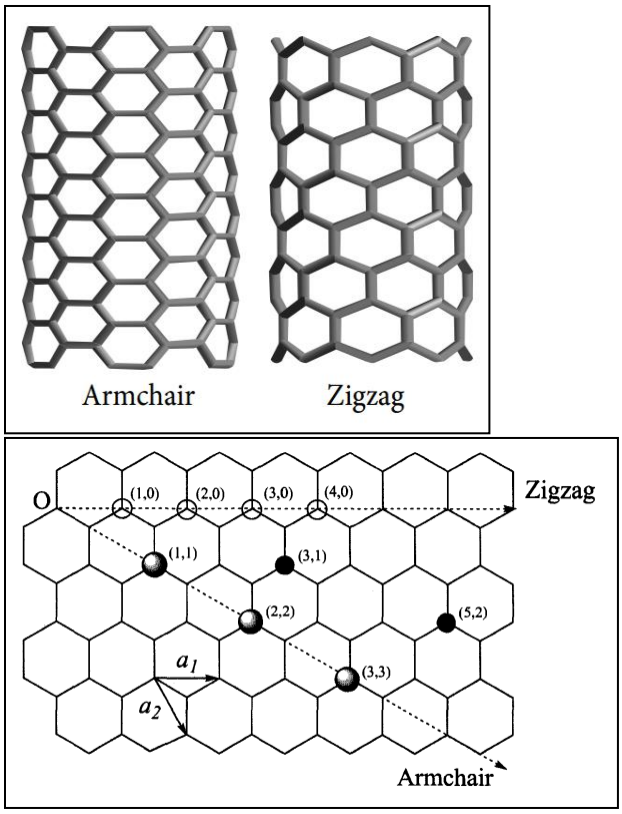


Figure 2. Graphene sheet showing coordinate system Schematic representation of the relation between nanosheet and nanotubes [16]

Based on "equation 2", the diameter of the :CNT can be calculated such that

$$D_{CNT} = \frac{a\circ\sqrt{m^2+mn+n^2}}{\pi} \qquad (2)$$

Where ao = 3 b denotes the length of the C-C bond, which is believed to be 0.142 nm [17].
The warpeing of the graphene sheet depends itself on the values of the pair of indices (n, m). In the graphene honeycomb crystal lattice, the integers n and m denote the number of unit vectors in each direction. When m = 0, nanotubes are referred to as zigzag nanotubes, and when n = m, they are referred to as armchair nanotubes or Chiral nanotubes. The diameter of an ideal nanotube can be measured as a = 0.246 nm using its (n, m) indices.

2.2. Finite element modeling

A 3D FE model has been developed in this study to determine the mechanical properties of SWCNTs. The commercial FE program ANSYS was used to create the 3D FE model. Nodes were mounted at the positions of carbon atoms to create the FE models. Three-dimensional elastic BEAM4 ANSYS modules were used to model the covalent bonds between them. Two nodes, The cross-sectional area, two moments of inertia, two dimensions, and material properties describe this function. At each node, there are six degrees of freedom. The bond length L and the wall thickness t refer to the element length L and the element diameter, respectively, as a consequence of this experiment Make a single ring to begin modeling a CNT, then repeat the process along the central axis to finish the structure. Unit cells are replicated around the central axis to form the ring. Figure 3 depicts the geometry of unit cells.

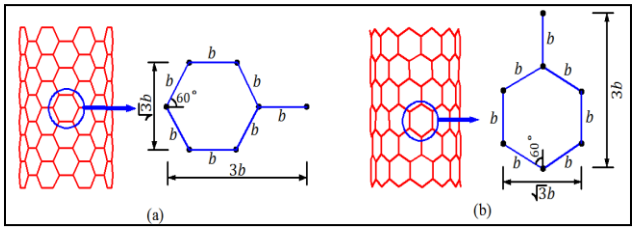


Figure 3. Geometry of unit cell (a) Armchair (b) Zigzag

In order to simulate unit cells, computer-aided design software (ANSYS) was used to first determine the coordinates of each carbon atom. The atoms would then be connected with each other in order to build the hexagonal unit cell. To make a single loop, the unit cells were replicated around the central axis. Finally, the single ring can be repeated around the CNT's central axis. a SWCNT can be constructed. Fig. 4 shows the required steps for representing the SWCNT using the ANSYS software.

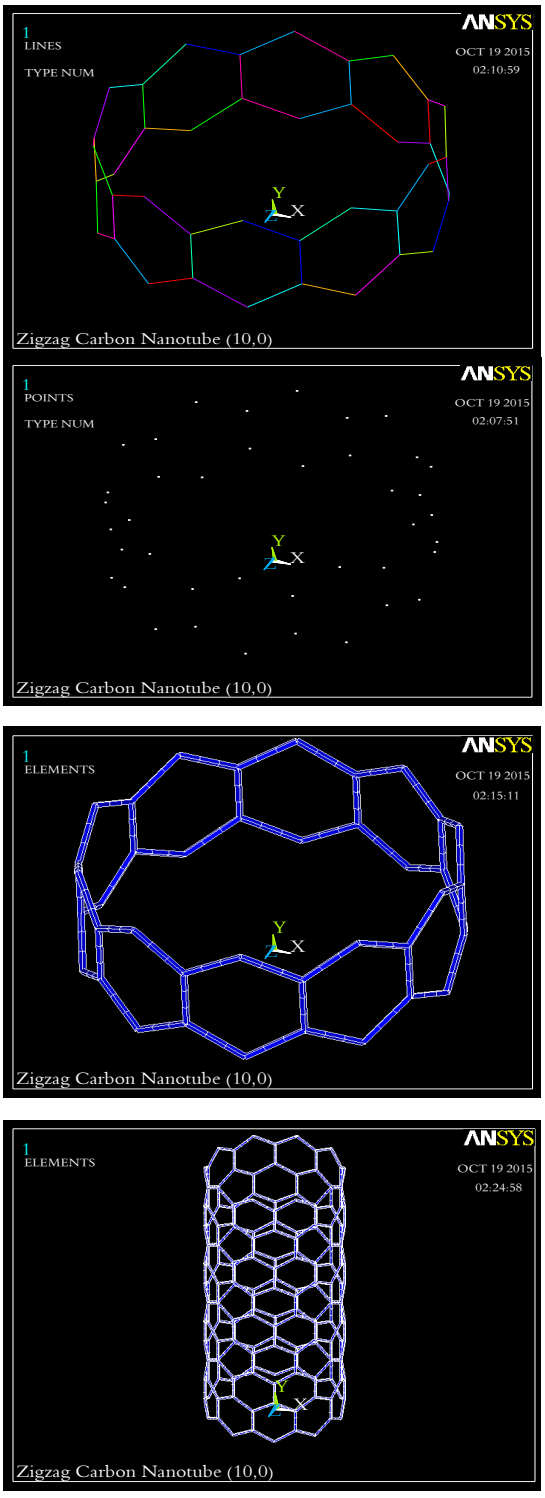
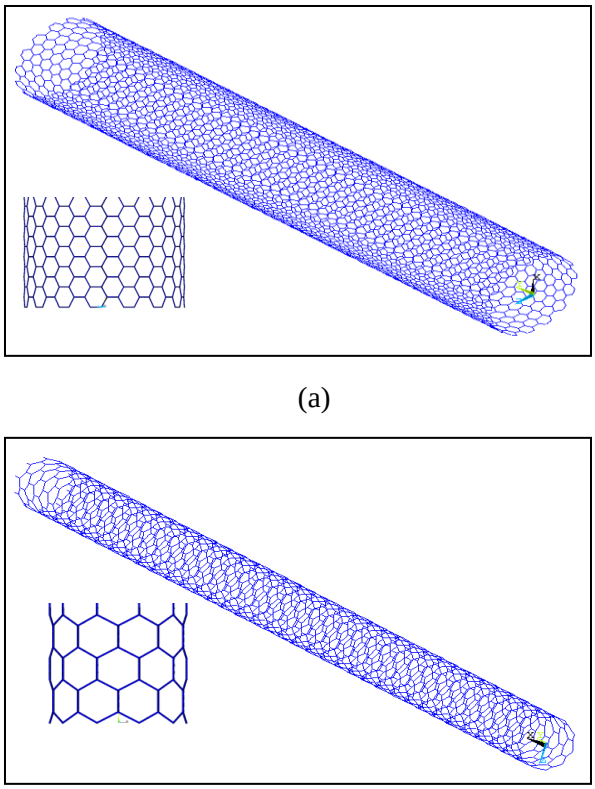


Figure 4. Finite element model of zigzag CNT structure using ANSYS software.

As a next step, the model will be meshed and loaded with boundary conditions as shown in Fig. 5 and Fig. 6 respectively.



(a)

(b)

Figure 5. The FE meshes of the (a) Armchair (15, 15), and (b) Zigzag (10, 10) SWCNTs.

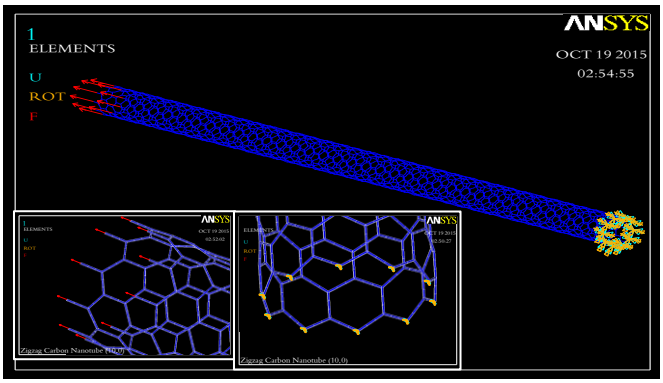


Figure 6. The applied boundary conditions on the nanotube SWCNTs.

Strong mechanics and molecular mechanics principles are used to explain C-C bonds. The required properties are obtained using a force field constants approach and an energy approach. The conditions and element properties used in this investigation are described in Table 1.

Table 1. Covalent bonds between carbon atoms have material and geometric properties [18].

Corresponding force field constants	k_r = 651.97 nN/nm
	k_θ = 0.8758 nN nm/rad^2
	k_φ= 0.2780 nN nm/rad^2
$E =$ Young's modulus $= \frac{kr^2 b}{4\pi k_\theta}$	5.484 $\times 10^{-6}$ N/nm^4
$R_b =$ bondradius $= 2\sqrt{\frac{k_\theta}{kr}}$	0.0733 nm
$I_{xx} = I_{yy}$ $= second\ moments\ of area$ $= \frac{\pi {R_b}^4}{4}$	2.2661 $\times 10^{-5}$ nm^4

4. Results and Discussion

The commercial finite element program ANSYS is used to model twelve single wall carbon nanotubes in this analysis. The thickness is assumed to be 0.34 nm in all configurations [19]. The boundary conditions are used to calculate the elastic modulus of CNTs. On one end of the structure, each node's degrees of freedom are arrested, and an axial force is applied to each node on the other. The Modulus of elasticity of CNTs is determined using one-dimensional Hooke's law and the corresponding equations:

$$\sigma = stress = \frac{P}{A} = (\frac{reaction\ forc}{cross-sectional\ area}) \quad (3)$$

$$\varepsilon = strain = \frac{\Delta L}{L} = \frac{/displacement}{length\ of\ CNT}) \quad (4)$$

$$E = Young's\ modulus = \frac{\sigma}{\varepsilon} \quad (5)$$

4.1. SWCNTs' Young's modulus

The Young's modulus of a material is the ratio of normal stress to normal strain obtained from a uni-axial tension test (= E). Since this study was carried out in a linear region. The original length of the CNT is Ao= L o, and the original cross-section area is Ao= L o. and L is the displacement applied, where d is the diameter of the CNT and t is the thickness of a SWNT. F is the total tensile force applied, and Ao=dt was calculated (where d is the diameter of the CNT, t is the thickness of a SWNT), L ois the original length of the CNT, and L is the Table 2 lists the characteristics of testedSWNTs.

Table 2. Characteristic of simulated SWCNTs.

CNT Type	Chirality (n, m)	Diameter (nm)	Length (nm)	L/D	layers	Young modulus TPa
Armchair CNTs	(4,4)	0.542	12.3	22.69	50	1.0278
	(6,6)	0.814	12.3	15.11	50	1.0281
	(8,8)	1.085	12.3	11.34	50	1.0282
	(10,10)	1.356	12.3	9.07	50	1.0283
	(13,13)	1.763	12.3	6.97	50	1.0284
	(15,15)	2.034	12.3	6.05	50	1.0285
Zigzag CNTs	(5,0)	0.391	12.354	31.59	29	0.9909
	(8,0)	0.626	12.354	19.73	29	1.0191
	(10,0)	0.783	12.354	15.77	29	1.0238
	(15,0)	1.174	12.354	10.52	29	1.0292
	(20,0)	1.566	12.354	7.89	29	1.0361
	(25,0)	1.957	12.354	6.31	29	1.0396

Of importance, all the numerical simulations have been validated due to the data obtained from literatures shown in Table 3. The selected results from literatures include Li and Chou [20] , Lu [21] , Hernandez et al. [17] , Jin and Yuan[22] ,Yu et al. [9] , Tombler [13], Salvetat et al.[11] Krishnan et al.[6] Shokrieh and Rafiee [23] Meo and Rossi [24] , Giannopoulos et al. [25].

Table 3. Comparison of Young's modulus CNT Young's modulus reported by different researchers.

Investigator	Method	Young's Modulus (TPa)
Li and Chou [20]	Structural mechanics	1.01
Lu [21]	Molecular Dynamics	0.974

Hernandez et al. [17]	Molecular Dynamics	1.24
Jin and Yuan [22]	Molecular Dynamics	1.238
Yu et al. [9]	Experimental	0.32–1.47
Tombler [13]	Experimental (AFM)	1.2
Salvetat et al. [11]	Experimental	0.8–1.21
Krishnan et al. [6]	Experimental	0.9–1.7
Shokrieh and Rafiee [23]	continuum mechanics	1.04
Meo and Rossi [24]	Nonlinear FEM	0.92
Giannopoulos et al. [25]	Linear FEM	1.248
Present work	Linear FEM	0.99–1.039

4.2. SWCNT Young's modulus as a function of diameter

Based on significance considerations, the FE model .the effect of diameter on the elastic modulus of SWCNTs was investigated using this method.This investigation took into account two forms of SWCNTs: zigzag and armchair The difference in the Young's modulus versus the CNT diameter for the armchair and zigzag SWCNTs, respectively, is plotted in Fig. 7. As can be shown, the diameter has a major impact on the Young's modulus in both armchair and zigzag SWCNTs. Hence, increasing the tube diameter can significantly increase the Young's modulus for all cases of SWCNTs in general. Although, the trend increment might be different for each considered diameter in the cases of SWCNTs.

In fact, the Young's modulus of SWNCTs is obviously found to be influenced by relatively smaller diameters rather than when larger diameters are considered. This might be explained due to the fact that, the curvature of CNTs is varied when the diameter is changed. Or in other word, in smaller diameters the curvature of CNT is in general greater than that in larger diameters. Therefore, the distortion in C-C bonds for small diameters of CNT observed to show more effects on Young's modulus. In another word, when the diameter increases the effect of curvature decreases gradually as a result.

However, in the case of armchair and when the diameter is ranged from 0.542 nm to 2.03 nm the Young's modulus value has been observed to vary from 1.0278 to 1.0285 TPa. Wherein, in zigzag SWNTs the Young's modulus value is approximately obtained to be from 0.391 to1.957 TPaas the diameter ranged from 0.9909 to 1.0396 nm.

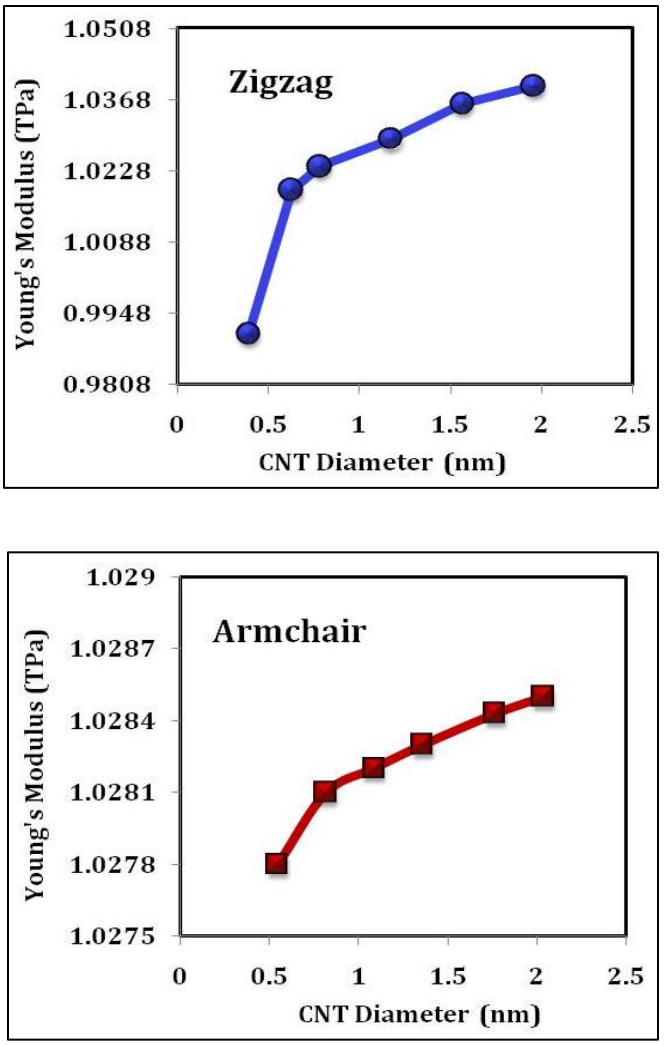
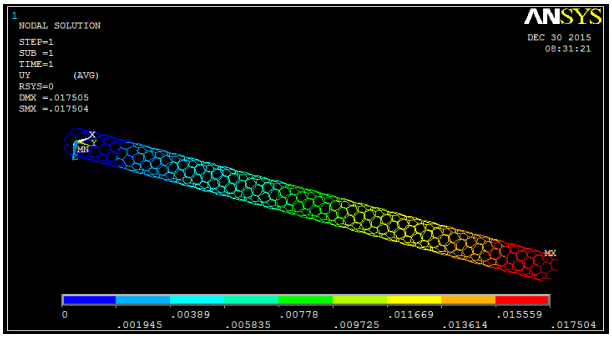


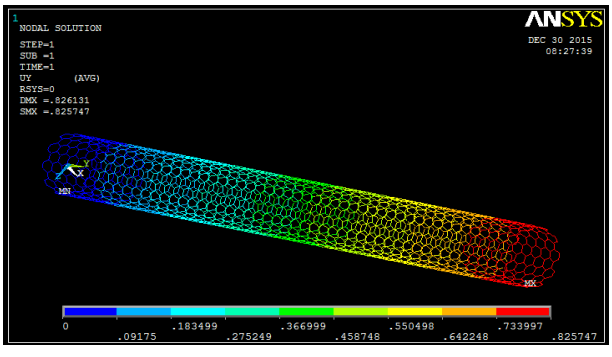
Figure 7. Young's modulus for armchair and zigzag configurations as a function of nanotube diameter.

4.3. Effect of length to diameter ratio (L/d) in SWCNTs

In this study, the impact of the length to diameter ratio (L/d) on Young's modulus was also observed for armchair and zigzag. As seen in Figure, (10, 10) armchair and (8, 0) zigzag single wall carbon nanotubes were chosen for this reason (8). The effect of the length to diameter contrast ratio of these nanotubes is shown in Table 4.Fig. 8 a and Fig. 8 b show the obtained variation in the young modulas due to the change in l/d ratio for the armchair and zigzag carbonnano tubes respectively. Fig. 9 a showed that, in armed chair mode the increase in the l/d ratio can lead to a dramatic increment in the young moduals value. Wherein Fig. 9 b showed that, the change in the aspect ratio has no serious effect on the mechanical ability of the nanotube, even when high values of the aspect ratio are considered.



(a)

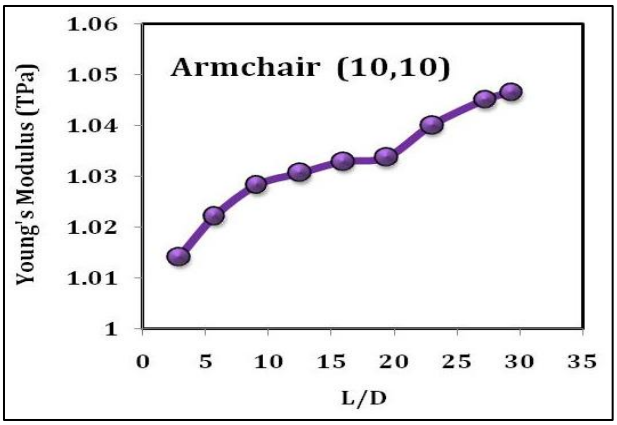


(b)

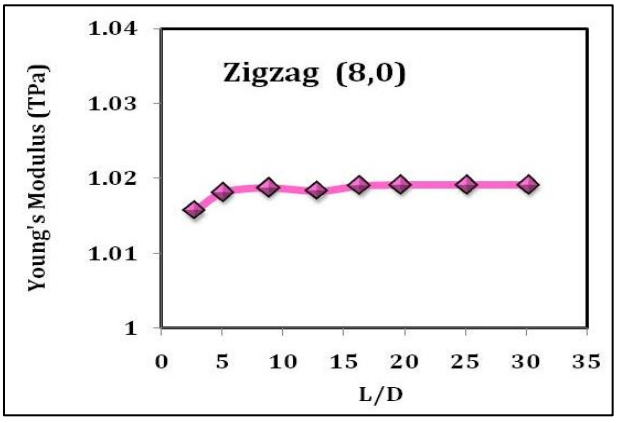
Figure 8. Deformed shape of a single-walled carbon nanotube of (a) Armchair (10, 10) (b) Zigzag (8, 0)

Table 4. Influence of aspect ratio (L/D) on modulus (E)

SCN Type	Diameter (nm)	L/D Ratio	Young's Modulus (TPa))
Armchair (10,10)	1.356	3	1.0141
	1.356	6	1.0221
	1.356	9.0707	1.0283
	1.356	12.5	1.0307
	1.356	16	1.0329
	1.356	19.5	1.0337
	1.356	23	1.0400
	1.356	27	1.0451
Zigzag (8,0)	0.626	2.5	1.0157
	0.626	5	1.0181
	0.626	9	1.0187
	0.626	13	1.0183
	0.626	16	1.0190
	0.626	19.73	1.0191
	0.626	25	1.0191
	0.626	30	1.0191



(a)

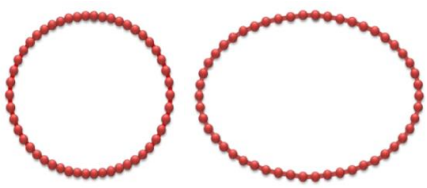


(b)

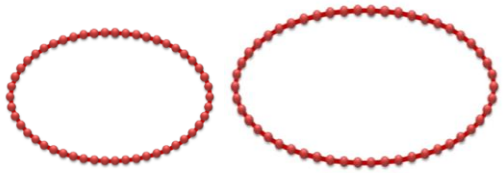
Figure 9. Variation of Young's modulus of (a) Armchair (10,10) and (b)Zigzag (8, 0) with different length to diameter ratio.

4.4. Effects of cross sectional aspect ratio (a/b) on the elastic moduli of SWCNTs

As a next step attached to this work, (15, 15) armchair and (25, 0) zigzag single wall carbon nano-tubes has been considered herein. Fig. 10 shows Cross sections of elliptical single wall carbon nano-tubes (ESWCNTs) for different a/b values; i.e. from1 to 2. Table 5 lists the values of young's moduli in terms of the change in the geometry of SWCNT. Figure 11 demonstrates how the elastic moduli of armchair and zigzag SWCNTs change as the sectional aspect ratio (a/b) changes. For both armchair and zigzag SWCNTs, it can be shown that this parameter has a significant impact on the Young's modulus. In fact, increasing the cross sectional aspect ratios (a/b) can lead to considerable reduction in the elastic moduli. The figures suggested that, the elastic moduli values are inversely proportional to the cross sectional aspect ratio. Frantically, the elastic moduli of ESWCNTs are observed to be smaller than their values in comparison to SWCNTs. As a result, changing the geometry of SWCNTs leads to decrease their elastic moduli or in other word any change in the geometry operates as a defect and decreases the elastic moduli. However, maximum value of Young's Modulus for the armchair model has been obtained to be 1.0285 TPa when the aspect ratio is 1. In the same vein the maximum value Young's Modulus for the zigzag models has reached 1.0396TPa when the aspect ratio is 1



a/b = 1 *a/b = 1.25*



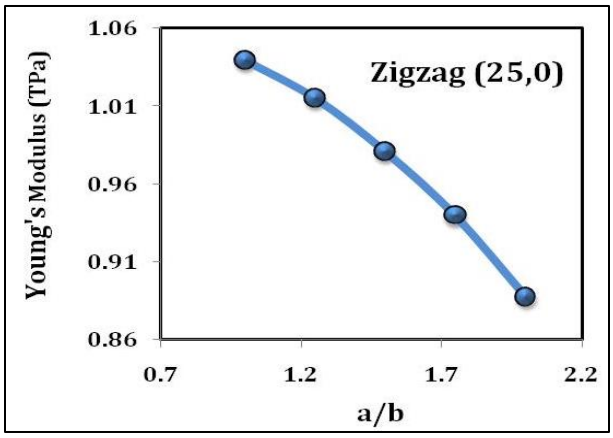
a/b = 1. 5 *a/b = 1.75*

a/b = 2

Figure 10. Cross sections of SWCNTs for different a/b

Table 5. Influence of aspect ratio (a/b) on Young's modulus (E)

SCN Type	cross section Area (nm^2)	a/b Ratio	Young's Modulus (TPa)
Armchair (15,15)	2.1730	1	1.0285
	2.1730	1.25	1.0114
	2.1730	1.5	0.9613
	2.1730	1.75	0.8864
	2.1730	2	0.7991
Zigzag (25,0)	2.0910	1	1.0396
	2.0910	1.25	1.0152
	2.0910	1.5	0.9813
	2.0910	1.75	0.9421
	2.0910	2	0.8873



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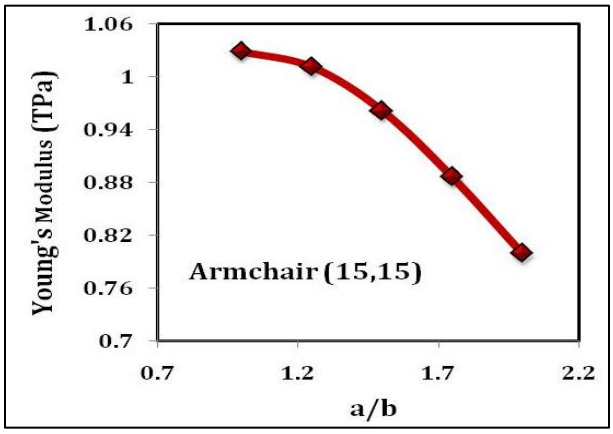


(b)

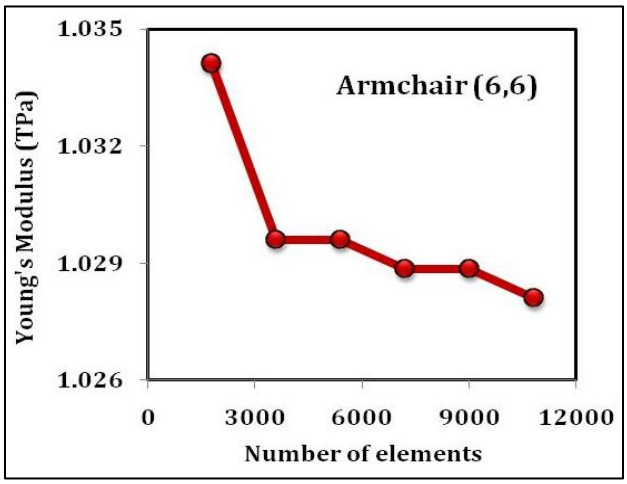
Figure11. Variation of Young's modulus of (a) Armchair (15, 15) and (b) Zigzag (25, 0) with the (a/b) aspect ratio.

4.5. Effect of number of element on SWCNTs

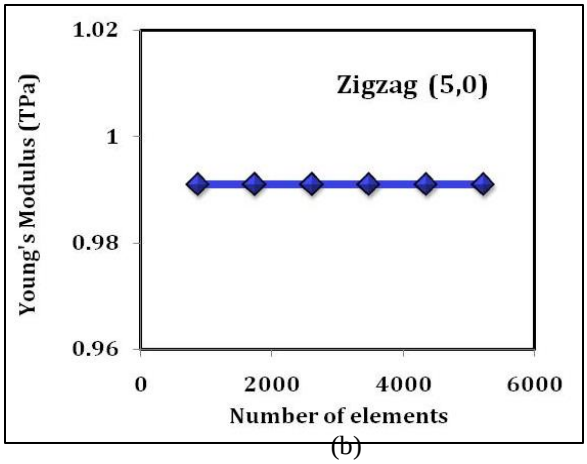
Two versions of (6, 6) armchair and (5, 0) zigzag have been designed to investigate the impact of meshing on the young's modulus of SWCNTs. Table 6 lists the number of elements and nodes for each model wherein Fig. 12 shows the effect of number of elements on young's modulus for both models of SWCNTs. Fig. 12 a showed that, for armchair type of SWCNT a considerable effect in the young's modulus can be obtained in terms of increasing the number of the elements. This might be explained due to the fact that, increasing the number of elements can lead to increase the number of nodes that exposed to the applied load as well. Fig.12 b indicated that in the model of zigzag SWCNT, there is no recognized effect in the young's modulus when the number of elements is increased. Because in the zigzag model the number of nodes that exposed to the applied load will remain constant even when the number of elements is increased.

Table 6. List of number of elements for Armchair (6, 6) and Zigzag (5,0).

SCN Type	Length	No. of element	No. of nodes	Young's Modulus (TPa)
Armchair (6,6)	12.3	1806	1212	1.0341
	12.3	3612	3018	1.0295
	12.3	5418	4824	1.0295
	12.3	7224	6630	1.0288
	12.3	9030	8436	1.0288
	12.3	10836	10242	1.0280
Zigzag (5,0)	12.354	870	585	0.9909
	12.354	1740	1455	0.9909
	12.354	2610	2325	0.9909
	12.354	3480	3195	0.9909
	12.354	4350	4065	0.9909
	12.354	5220	4935	0.9909



(a)



(b)

Figure12. Effect the number of elements on Young's modulus of (a) (6, 6) armchair (b) (5, 0) zigzag

5. Conclusions

A finite element simulation technique for SWCNTs has been developed by ANSYS software. According to the modeling of armchair and zigzag of SWCNTs, the results extended to the considered design stated that any increasing in the diameter can lead to increase the elastic young modulus as a result. Furthermore, to this, It could be inferred that smaller diameters have a greater impact on the Young's modulus of SWNCTs than higher magnification. Whilst, the aspect ratio L/D does not seriously affect the modulus of elasticity of the SWCNTs. The increment in cross sectional aspect ratio (a/b) has led the elastic modulus to be decreased. Furthermore, the Young's modulus of armchair SWCNTs increases as the number of elements increases, while in zigzag SWCNTs, it remains constant as the number of elements increases.

Conflict of interest

The publication of this article cause no conflict of interest.

6. References

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