

## Methodology for Evaluating Theproperties of Carbon Nano Tubes for Engineering Applications

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### Abstract

Owing to the superior mechanical properties of Carbon Nanotubes (CNTs), research has been initiated to use this nanomaterial in construction industry. The elastic modulus of CNT is of great importance in order to use CNTs in construction industry. For judicious and effective application of CNT in construction industry where mass scale utilization is inevitable, it is important to accurately assess the properties of CNTs since these nano fiber materials are extremely cost sensitive. There is no well established tool or method available for the engineers to determine the properties of CNT, other than to accept the manufacturer's data. Nanoscale continuum theory uses a representative volume to determine the elastic modulus which does not include the effect of radius and aspect ratio. In the present study, numerical model is developed and the validated one is used to study the effects of geometrical variability's on the properties of CNT. Further, a methodology has been proposed to determine the mechanical properties, such as tensile stiffness, of the Carbon nanotube with a given structural arrangement (chirality and radius) if the same for the basic configuration, graphene, is known. The procedure discussed in this study will be helpful to the engineers to easily estimate the properties such as elastic modulus or tensile stiffness of CNTs before incorporating into conventional materials for developing new materials with enhanced properties.

**Keywords:** Carbon nanotube; Elastic modulu; Nanoscale continuum theory; Finite element analysis

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### Introduction

Carbon nanotube (CNT) is a cylindrical nanostructure which is envisioned as a roll of graphene sheet. The radius of the nanotube ranges from 0.3nm - 100nm and it has a very high aspect ratio. CNT may be single walled (SWNT) or multi-walled (MWNT). Iijima<sup>[1]</sup> discovered the CNT while studying the carbon produced by arc evaporation of graphite in the helium atmosphere using High Resolution Transmission Electron Microscopy (HRTEM). Since then, various experimental and theoretical studies have been carried out by researchers around the world to determine its mechanical, chemical and electrical properties.

Ruoff and Lorrents<sup>[2]</sup> reported that CNTs possess superior mechanical properties and can be used as a potential reinforcing material to develop composites of desirable mechanical properties. Konsta-Gdoutos et al.<sup>[3]</sup> found that the macro and nano-properties of cement got enhanced by dispersion of MWNT using ultrasonic energy and use of surfactant. Experiments conducted by Tyson et al.<sup>[4]</sup> on cement reinforced by 0.1 and 0.2 weight percentage of CNTs showed that the flexural strength, ductility, strain to failure, elastic modulus and fracture toughness of the material also got increased.

The elastic modulus of CNT is of great importance for developing a composite material by adding CNTs. Various researchers carried out experimental studies based on techniques using HRTEM, Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) to determine the elastic modulus of SWNTs and MWNTs. The elastic modulus of CNT reported by each researcher is scattered and found to fall in a range of 1TPa to 6TPa. Treacy et al.<sup>[5]</sup> observed the thermal vibrations of MWNT in TEM and reported its elastic modulus to be in the range of 0.4 - 4.15TPa with an average of 1.8TPa. Characteristics of SWNT in room temperature were observed by Krishnan et al.<sup>[6]</sup> using Transmission Electron Microscopy and its elastic's modulus was found to vary in the range of 0.9 - 1.7TPa with an average of 1.25TPa. The elastic modulus of an individual MWNT was reported as 1TPa based on its cross sectional analysis in SFM (Scanning Force Microscopy)<sup>[7]</sup>. The cooling-induced compressive deformation of CNT was monitored by micro-Raman Spectroscopy by Lourie and Wagner<sup>[8]</sup> and the elastic modulus of SWNT and MWNT was derived to be in the range of 2.8 - 3.6 TPa and 1.7 - 2.4 TPa respectively. Tensile tests were conducted by pulling MWNT using AFM tips and its behavior was observed under Scanning Electron Microscope (SEM). The tensile strength and the stiffness of MWNT obtained by this method was 11-63 GPa and 0.27 - 0.95 TPa respectively <sup>[9]</sup>.

Many theoretical studies using molecular dynamics, tight binding methods and continuum studies were also carried out to determine the elastic modulus of CNT and it was found that there was a huge scatter in the reported values. Molecular dynamics simulation was carried out using<sup>[10,11]</sup> interatomic potential and the response of SWNT subjected to compression was studied and an empirical relationship was given by Cornwell and Wille<sup>[12]</sup> to determine the elastic modulus of the CNT with respect to its radius. Prylutskyy et al.<sup>[13]</sup> carried out molecular dynamics studies using potentials based on bond stretching and bond angle changes and determined the elastic modulus as 1.1 – 1.2 TPa. Analytical expressions were obtained by Popov and Van Doren<sup>[14]</sup> to determine the elastic modulus of different chiral nanotubes using Born's perturbation technique for a lattice - dynamical model. The elastic modulus of nanotube was reported in Vaccarini et al.,<sup>[15]</sup> as 1.26 TPa using non-orthogonal tight binding method.

In continuum mechanics studies carried out by Yakobson et al.,<sup>[16]</sup> CNTs were modeled as a thin shell, a beam or many truss members. The continuum shell model was used to study the behavior of CNT beyond the elastic limit. CNT was modeled as a beam and its elastic modulus was determined by measuring the resonant frequency and using modulus – frequency relationship<sup>[17]</sup>. Odegard et al.<sup>[18]</sup> used truss members to determine the effective bending rigidity of CNT using equivalent continuum method. Nanoscale continuum theories have been established which links the continuum models with atomic simulations. Quasi-continuum method was developed in which atomistic simulations were carried out near the deformations and continuum analysis was carried out far away from the deformations thereby reducing the redundant degrees of freedom<sup>[19]</sup>. A nanoscale continuum theory of fracture nucleation in SWNT was developed incorporating the interatomic potentials<sup>[20]</sup>.

The nanoscale continuum theory was applied by Zhang et al.<sup>[21]</sup> to study the linear elastic modulus of SWNT using multi-body interatomic potential and considering the non-centrosymmetric structure of CNT. It was observed that the elastic modulus of CNT determined by each method is found to vary and it lies in a range from 1 TPa to 6 TPa. It is difficult to conduct experiments at nanoscale and to establish atomistic studies because of the huge computational efforts and sophisticated instrumentations. Hence, a simplified mathematical model is developed to determine elastic modulus of CNT of armchair and zigzag tubes using nanoscale continuum theory developed by Zhang et al.<sup>[21]</sup> and a numerical model developed by Jalalahmadi and Naghdabadi<sup>[22]</sup>.

Though few researchers<sup>[23-25]</sup> have taken into account the geometry of CNT for analytical and atomistic computation of its mechanical properties, studies on the influence of geometric parameters, both local (such as chirality) and global (such as aspect ratio), of CNTs have not been paid considerable attention. However, for engineering applications, it is important to evaluate the properties of CNTs with different geometrical configurations for judicious and appropriate application in enhancing/engineering various types of composites. The representative volume taken to determine the elastic modulus does not take into account effect of

the geometry of the nanotube and its chirality. Hence, the tensile stiffness and so the elastic modulus of any type of CNT obtained by this method will be the same which is found to be incorrect and highly conservative as the advantage due to the curvature of the tubes will not reflect in the mechanical properties. But, in order to take the advantage of higher modulus of CNT compared to graphene for civil engineering applications the effect of curved structure and its chirality should be taken into account. Hence, a validated finite element model has been used to study the effect of various parameters like chirality, tube radius and aspect ratio on the elastic modulus of CNT. A methodology using interatomic potential is proposed for determining the tensile stiffness of CNTs with different geometrical arrangements.

### Geometry of Carbon nanotubes

Carbon nanotubes can be specified by two different parameters, viz., its length and chirality. Chirality of a carbon nanotube is specified by the multipliers of two base vectors in a chiral vector. A chiral vector is the one along which the graphene sheet can be rolled to form a carbon nanotube. A graphene sheet can be assumed to have two base vectors along two directions of its crystal lattice,  $\vec{a}_1$  and  $\vec{a}_2$  as shown in Figure: 1.

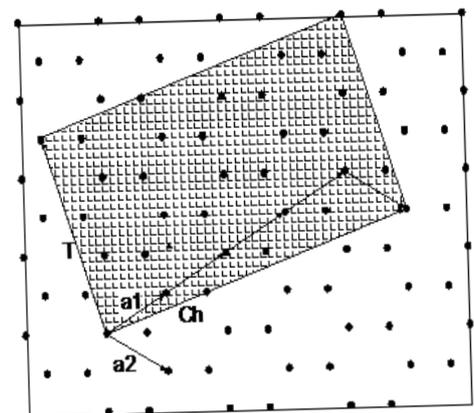


Figure 1. Unit cell of (4,1) nanotube

The chiral vector  $\vec{Ch}$  can be obtained by the summation of these two base vectors. Thus, the chiral vector is given by equation

$$\vec{Ch} = m\vec{a}_1 + n\vec{a}_2 \quad (1)$$

where m and n are the multipliers of the base vectors  $\vec{a}_1$  and  $\vec{a}_2$  respectively. In this case, the chirality of this nanotube is denoted as (m,n). There is another vector called translational vector  $\vec{T}$  which is perpendicular to chiral vector along the length of the nanotube defined as

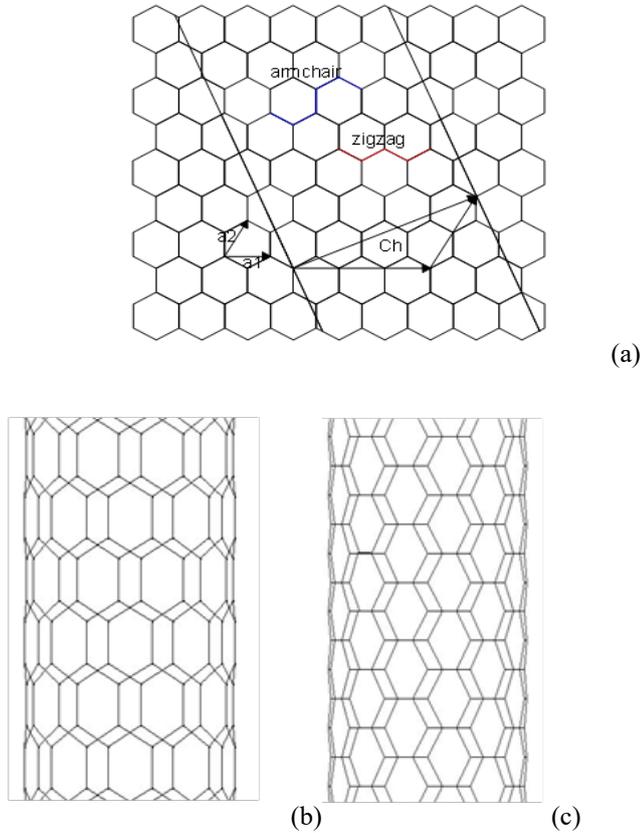
$$\vec{T} = t_1\vec{a}_1 + t_2\vec{a}_2 \quad (2)$$

where  $t_1 = \frac{2n+m}{d_R}$  and  $t_2 = -\frac{2m+n}{d_R}$  in which

$$d_R = \begin{cases} d, & \text{if } n - m \text{ is not a multiple of } 3d \\ 3d, & \text{if } n - m \text{ is a multiple of } 3d \end{cases} \quad (3)$$

And d is the highest common divisor of (n,m).

A rectangle bounded by vectors  $\vec{Ch}$  and  $\vec{T}$  forms a unit cell of a carbon nanotube. There are two common types of nanotubes based on the way the graphene sheet is rolled to form CNT; they are zigzag and armchair (Figure. 2).



**Figure 2.** a) Zigzag and Armchair formed from graphene sheet, b) Zigzag CNT c) Armchair CNT

If the chirality of nanotube is  $(n,0)$ , it is called zigzag nanotube and if it is  $(n,n)$ , it is called armchair nanotube.

Since the chiral vector is rolled to form a tube, the length of the chiral vector is equal to the circumference of the nanotube. The length of the chiral vector is given by,

$$L = \sqrt{3}l_0 \sqrt{n^2 + m^2 + nm} \quad (4)$$

where  $l_0$  is the carbon-carbon bond length in the graphene sheet which is 1.421Å.

Hence, the diameter of the nanotube is given by,

$$d = \frac{\sqrt{3}l_0 \sqrt{n^2 + m^2 + nm}}{\pi} \quad (5)$$

### Interatomic potential and nanoscale continuum theory

Interatomic potential of a bond denotes the potential energy stored in it under deformation. In order to properly capture the interatomic interactions of the carbon nanotube, it is insufficient to have an interatomic potential that accounts only the effect of change in the desired carbon-carbon bond length. The bond angle and the position of carbon atoms near the desired carbon-carbon bond should also be taken into account. Among many empirical interatomic potentials proposed for car-

bon-carbon bonds, the most widely accepted one is the Tersoff–Brenner<sup>[10,11]</sup> potential which takes into account these multi-body effects also.

The interatomic potential for a bond between two carbon atoms  $i$  and  $j$  was developed by Tersoff (1998) and Brenner (1990) and is given as

$$V_{ij} = V_R(r_{ij}) - B_{ij} V_A(r_{ij}) \quad (6)$$

Where  $r_{ij}$  is the distance between atoms  $i$  and  $j$ .  $V_R(r_{ij})$  and  $V_A(r_{ij})$  are repulsive and attractive pair potential terms which represent repulsive and attractive forces between atoms  $i$  and  $j$ .

A nanoscale continuum theory was proposed by Zhang et al.<sup>[21]</sup> by which the macroscopic deformation of the material can be linked to the interatomic potential and the atomic structure of the material. This is achieved through Cauchy-Born rule of crystal elasticity, by equating the strain energy of the material at the continuum level to potential energy stored in the bonds due to the imposed deformation. This is given by

$$W = \frac{1}{2\Omega_e} \sum_{i,j} V(r_{i,j}) \quad (7)$$

where  $W$  is the strain energy density of the representative cell and  $V(r_{i,j})$  is the interatomic potential of the atomic bond between atoms  $i$  and  $j$  which denotes the potential energy stored in it when it is subjected to deformation.  $\Omega_e$  is the volume of the representative cell which is equal to  $\frac{3\sqrt{3}}{4}l_0^2$  where,  $l_0$  is the outstretched length of a carbon-carbon bond in carbon nanotube. The factor  $\frac{1}{2}$  comes due to the equal splitting of bond energy to each atom.

From nanoscale continuum theory, the linear elastic modulus tensor can be obtained using,

$$C = \left[ \frac{\partial^2 W}{\partial E_G \partial E_G} - \frac{\partial^2 W}{\partial E_G \partial x} \left( \frac{\partial^2 W}{\partial x \partial x} \right)^{-1} \cdot \frac{\partial^2 W}{\partial x_G \partial E_G} \right]_{E_G=0, x=0} \quad (8)$$

Let  $Z$  denote the axial direction of SWNT and  $\theta$  denote the circumferential direction of SWNT. The non-vanishing terms of the linear elastic modulus tensor are  $C_{ZZZZ}$ ,  $C_{\theta\theta\theta\theta}$  and  $C_{ZZ\theta\theta} = C_{\theta\theta ZZ}$ . Hence, for a simple tension along the axial direction of SWNT, the elastic modulus is given by

$$E_{inter} = C_{ZZZZ} - \frac{C_{ZZ\theta\theta}^2}{C_{\theta\theta\theta\theta}} \quad (9)$$

The elastic modulus tensor and the linear elastic modulus obtained are actually the tensile stiffness, i.e., modulus multiplied by thickness rather than the modulus. By using Eqn. (9), linear elastic tensile stiffness of CNT with interatomic potential given by Brenner<sup>[11]</sup> is obtained as 159N/m. This value was proposed as the tensile stiffness of CNTs when the effect of curvature is not taken into account. In the present study, the same is used to normalize the results obtained for tensile stiffness of CNTs by considering the effect of curvature (discussed in section 5).

## Numerical simulation

The linear elastic tensile stiffness as obtained above does not depend upon the chirality of the nanotube and the tube radius. In order to find out the dependence of elastic modulus of SWNT on parameters like chirality, tube radius and the aspect ratio, a study has been carried out on the numerical simulation of carbon nanotube. A 3-D Finite Element Model was created in ANSYS in which nodes were placed in the location of carbon atoms and the covalent bonds between the carbon atoms were replaced by three dimensional BEAM 4 elements. BEAM4 element has six degrees of freedom and is defined by two nodes as well as its cross-sectional area, two moments of inertia, two dimensions and material properties.

From classical mechanics, the stretching stiffness,  $K_F$  and the bending stiffness,  $K_M$  of the beam are as follows:

$$K_F = \frac{EA}{1} \quad (10)$$

$$K_M = \frac{EI}{1}$$

Jalalahmadi and Naghdabadi<sup>[22]</sup> used Morse potential in which the parameters were changed to fit the Brenner potential and obtained the effective stretching and bending stiffness of the bond as 854 nN/nm and 0.9nN.nm/rad<sup>2</sup>, respectively. Using these values and assuming circular cross-section, the diameter of the beam element is found to be 0.1296 nm and the material used as beam element is found to have the elastic modulus as 9.382TPa. Since the model is in linear regime, the strain energy,  $U$  of the SWNT is given by

$$U = \frac{1}{2} \sigma \varepsilon AL$$

$$= \frac{1}{2} E \varepsilon^2 AL \quad (11)$$

Where  $\sigma$  is the stress,  $\varepsilon$  is the strain,  $E$  is the elastic modulus,  $L$  is the length of the nanotube and  $A$  is the area which is equal to  $\pi Dt$  in which  $D$  is the diameter and  $t$  is the thickness of the tube. From this, the elastic modulus of the nanotube can be obtained as

$$E = \frac{2U}{AL\varepsilon^2} \quad (12)$$

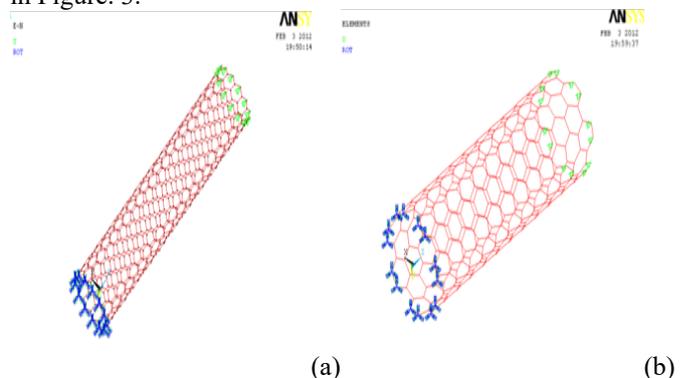
A Finite Element model of SWNT of particular diameter and length with the properties as described above is generated in ANSYS software. It is fixed at one end and stretched at the other end thereby producing tensile strain. The total strain energy,  $U$  of the SWNT is calculated by summing up the strain energies of each beam element of the generated model and the elastic modulus is calculated using the above expression. It can be found from Table 1 that the elastic modulus of the SWNT obtained from the present study using the Finite Element Modelling agrees well with the results reported in Jalalahmadi and Naghdabadi<sup>[22]</sup>

Chirality	Elastic modulus (TPa)	
	Present study	Reported in literature [Jalalahmadi and Naghdabadi (2007)]
(7,7)	3.34	3.296
(12,0)	3.312	3.312
(5,9)	3.392	3.514

**Table 1.** Validation of the Elastic modulus of CNT obtained from the present study

From Table 1, it can be observed that the values obtained in the present work are in good agreement (within 5% deviation) with that reported in the literature. Since the thickness of SWNT is of an atom thick, it is more meaningful to determine the tensile stiffness rather than the elastic modulus of the nanotube. Tensile stiffness of the CNT is obtained by dividing the elastic modulus of the tube by the thickness of the tube.

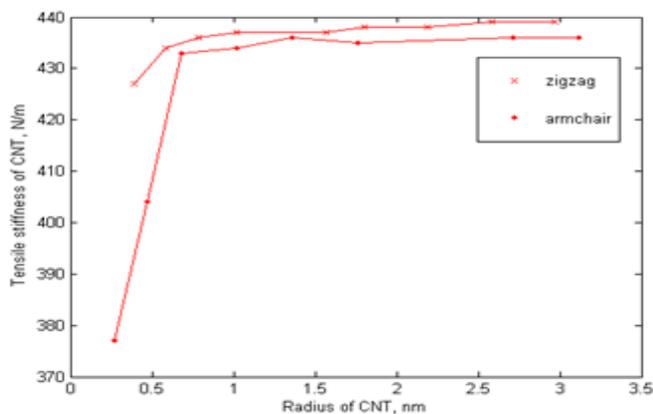
**Study on various parameters:** The validated Finite Element Model is used to study the effects of nanotube radius, aspect ratio and chirality of SWNT on its tensile stiffness. The effect of change in radius of the nanotube on the tensile stiffness for two different chiral tubes, viz., zigzag ( $n, 0$ ) and armchair ( $n, n$ ) was studied. The radius of the nanotube was varied from 0.3nm to 3nm keeping the aspect ratio constant equal to 6 in both the cases. The tensile stiffness of the nanotube was plotted with respect to the tube radius for two different chiral tubes which is shown in Figure. 3.



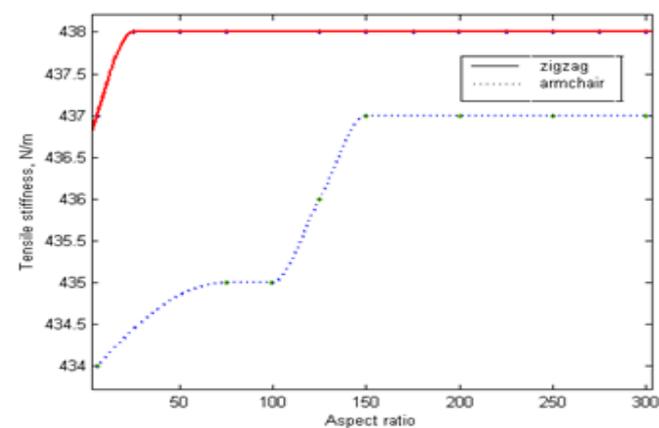
**Figure 3.** Finite Element model of a) (10,0) and b) (7,7) CNT

It is seen from the plot that the tensile stiffness of zigzag nanotube was 13% greater than armchair when the radius of the tube was 0.3nm. The difference in tensile stiffness of both the tubes decreased gradually up to the radius of 0.8nm. For nanotubes of radius greater than 0.8nm, the difference in percentage of tensile stiffness of CNT reduced to 0.7%, i.e., almost remained equal. This shows that the tensile stiffness of nanotubes of radius greater than 0.8nm is independent of tube radius and its chirality. It is to state the variation in the tensile stiffness of CNTs with small radius is due to the difference in force transfer mechanism in both types of CNTs. When the radius is less, owing to the local distribution of nodes for application of loads at the ends of the CNTs, armchair results in more displacement in comparison with the zigzag ones. However, with the increase in radius (aspect ratio has been kept constant), presence of nodes to distribute the applied load increases and thus, the influence of local geometrical distribution of nodes at the section of ap-

plication of loads, on global response such as stiffness of the CNTs reduces which is clearly depicted in Figure. 4. The effect of change in aspect ratio of the nanotube on the tensile stiffness for both the chiral tubes was also studied using the validated Finite Element Model. The aspect ratio of both the chiral tubes was varied from 6 to 300 keeping the radius of the tube constant equal to 1nm in both the cases. The tensile stiffness of the nanotube was plotted with respect to its aspect ratio for both the cases as shown in Figure. 5. It is significant to note that the behavior is presented only for a certain range for bringing out the clarity and better understanding. Though, it is apparent from the figure that the variation of tensile stiffness among zigzag and armchair is large, quantitatively it is not so. For example, the maximum variation in tensile stiffness among both types of CNTs is found to be less than 1%. Also the sudden increase in tensile stiffness observed in armchair nanotube is due to the numerical convergence (tensile stiffness of 435 to 437 N/m). Hence it is evident that the tensile stiffness is independent of aspect ratio of the tube.



**Figure 4.** Tensile stiffness vs radius of CNT for armchair and zigzag

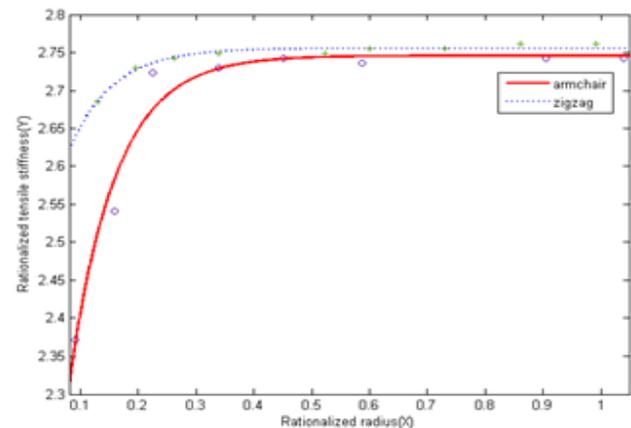


**Figure 5.** Tensile stiffness of CNT vs aspect ratio for armchair and zigzag CNTs

### Determination of the tensile stiffness of carbon nanotube

From the above studies, it has been found out that the tensile stiffness of nanotube varies with respect to the radius of the tube, its chirality and is independent of the aspect ratio of the tube. Hence, a methodology to obtain the tensile stiffness of the nanotube of a particular chirality and tube radius which also involves the interatomic interactions has been worked out. To maintain the dimensionality, the tensile stiffness is normalized as the ratio of the obtained tensile stiffness to the tensile stiffness which accounts only the interatomic interactions and the radius is nor-

malized with respect to the maximum radius taken for the study. A curve is fitted between the normalized tensile stiffness and the normalized radius and shown in Figure.6.



Normalized tensile stiffness and normalized radius

This plot is curve fitted and an expression is obtained. The  $R^2$  value of the fitted curve is 0.9719 and 0.9688 for zigzag and armchair respectively. From the curve, the tensile stiffness of different chiralities and diameters can be determined. From the above study, it has been observed that,

$$E = f(E_{inter}, r, \text{chirality}) \quad (13)$$

It is to underscore that the study is carried out with limited number of cases and few key variables. For developing the unified solution or proposing a closed form relation among the variables with the tensile stiffness of CNTs, a large space of samples needs to be investigated and analyzed. The scope of this work is limited to evaluation of mechanical properties of defect free CNTs whereas market available and fabricated CNTs are bound to have defects. With different types of defects, further studies are to be carried out for more generalized results. However, in the current work authors have limited their observations only to the defect free ones in order to understand the influence of geometrical parameters on the mechanical characteristics of CNTs in detail which would otherwise bring confusion why a particular phenomenon has been observed if the defects were also considered. The present study has been limited to CNTs of two different chiralities, viz., armchair and zigzag. It is found that the local geometrical arrangement play a role on the mechanical behavior of the CNTs. Extrapolation of these observations to CNTs with other chiralities would be over simplification and could be erroneous as well. Therefore, it is to mention that the study on mechanical behavior of other chiral tubes needs further study.

### Conclusion

The present study presents a methodology for determining the tensile stiffness of CNTs. With the known properties of graphene, it is attempted to provide the information on the mechanical properties of CNTs with different geometries by bridging the knowledge on interatomic potentials with FEM. From the study, it is found that:

1. The tensile stiffness obtained is approximately three times higher than the tensile stiffness obtained by considering the flat configuration. This increase is attributed to the curvature of graphene to form a CNT.

2. The elastic modulus of the nanotube depends on the chirality of the tube. The elastic modulus of the zigzag nanotube is higher than that of armchair nanotube of same radius.
3. The elastic modulus of both the chiral tubes of particular radius is independent on the aspect ratio of the tube.
4. The elastic moduli of both the chiral tubes depend on the radius of the tube up to 0.8nm and remains constant after that.

A methodology has been proposed by using the interatomic potential to determine the tensile stiffness of the nanotube where the chirality and radius of the nanotube are the also the parameters. The methodology proposed in the present study will be helpful to the engineers to easily estimate the properties of CNTs for developing new CNT based improved materials. Further studies are being carried out to determine the mechanical properties of CNT modified cementitious composites where the observations presented here will be extremely useful.

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