

# Evaluation of Tensile Modulus of Carbon Nanotube Bundle Based Composite with Interface Using Finite Element Method

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**Abstract:** Carbon Nanotubes (CNTs) have remarkable mechanical, thermal and electrical properties. The properties of CNTs depend on atomic arrangement (how the sheets of graphite are rolled), the diameter and length of the tubes and morphology of nanostructure. In this paper effective elastic properties of CNT based polymer composites are evaluated using a square Representative Volume Element (RVE) in finite element method (FEM). COMSOL Multiphysics 3.5 is used for making the models and doing simulations. Tensile modulus of a Single CNT based polymer composites are evaluated analytically and validated by simulation technique. The effect of varying CNT diameter and length on elastic properties of CNT reinforced composites is estimated and analyzed. In every model an interface is used between matrix and CNT.

**Keywords:** Bundle based Carbon Nanotube, COMSOL Multiphysics 3.5, CNT, FEM, RVE, Interface.

## 1. Introduction

Carbon nanotubes (CNTs) possess extremely high stiffness, strength, and resilience which can be the ultimate reinforcing materials for the development of nanocomposites. However, the nanotube dimensions of the order of a few nanometers in diameter and a few hundreds of microns in length have put huge unsolved challenges before researchers. Many believe that CNTs may provide the ultimate reinforcing materials for the development of a new class of nanocomposites. The elastic properties and load carrying capacities of CNTs in nanocomposites have been demonstrated in several research works. Some of these investigations show that the load-carrying capacity of CNTs in a matrix as well as the improvement of the elastic properties of the composites is significant and the CNT-based composites have the potential to

provide extremely strong and ultra light new materials.

In the production processes, it is difficult to get isolated CNT. CNTs have a propensity to aggregate to bundle or wrap together due to high surface energy and surface area and they are used in composite in this bundled form. Compared to the researches done on isolated CNT based composites, there are not much works on CNT bundle based composites. However, there are few studies regarding the mechanical characterization of the CNT bundle based polymer composites.

There are many simulations done on Single CNT based composites. And it is easy to verify those results by 'Rule of Mixtures' which is used for long Single CNT and formulas [9] which is used for short Single CNT. But those methods do not include the effect of interface. Moreover, in case of bundle based composites there are neither enough simulations nor a formula being established to evaluate elastic properties.

From the earlier studies it is seen that there is a wide variation in the reported elastic properties. Reported improvements in the elastic moduli are lower than the expected if the CNTs are assumed to act as reinforcing elements with an elastic modulus of 1 TPa. Discrepancies in the reported elastic moduli as well as in the strength of the CNT based polymer composites may be due to the insufficient load transfer through the interface between the CNT and the polymer matrix of the composites. Load transfer through the interface is affected by several factors. One of the vital factors is the morphology of the CNT bundle (i.e., agglomerated CNTs). Therefore it is necessary to investigate the effect of the morphology of the CNT bundle on the mechanical behavior of the CNT bundle based composites to fully realize the potentials of the CNT-based composites in real engineering applications.

Here a model of a Single CNT is developed and its different properties are evaluated and compared by the values obtained by "Rule of

Mixture”. In this model there is an interface whereas the “Rule of Mixture” does not consider the interface. After validation the effect of bundle diameter for both long and short CNT on the elastic properties of the CNT bundle reinforced polymer (with interface) composite is investigated using FEM. Also the effect of fiber length for short CNT on the elastic properties of the CNT bundle reinforced polymer (with interface) composite is investigated using FEM. Here all the models are developed and simulations are done using COMSOL Multiphysics 3.5

## 2. Representative Volume Element (RVE)

Concept of unit cells or representative volume elements (RVEs) which have been applied successfully in the studies of conventional fiber-reinforced composites at the microscale can be extended to study the CNT-based composites at the nanoscale. In the present study 3D nanoscale square RVEs are employed to investigate the various effects on the elastic properties of nanocomposites. The RVEs of single CNT based composite (Figure 1.) and CNT bundle based composite (Figure 2.) are shown.

The RVE used for analyzing long CNT bundle based/ long single CNT based composite has a length,  $L = 10\text{nm}$ . Only difference is the CNT is embedded through out the length in one of the corners in case of bundle based CNT composite whereas in single CNT based composite the CNT is in the middle of the composite. The diameter ( $d_c$ ) of the CNT is varied according to the chiral indices ((10, 10), (15, 15), (20, 20)) and so is the cross section of the composite (width =  $a$ ) to keep the CNT volume fraction to 5%.

In case of both long single CNT and long bundle based CNT, the length of the CNT is taken 10 nm. But to observe the effect of fiber length in case of short bundle based CNT the length is changed from 2.5 nm to 7.5 nm.

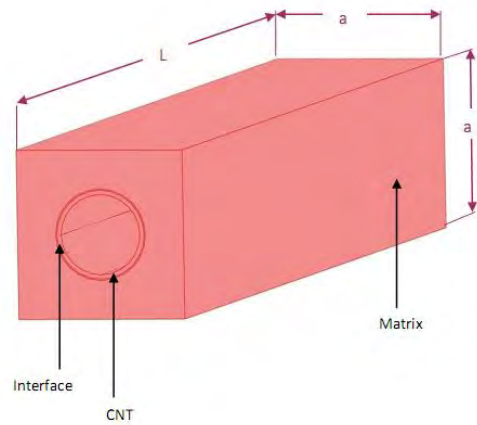


Figure 1. RVE for long CNT based composite

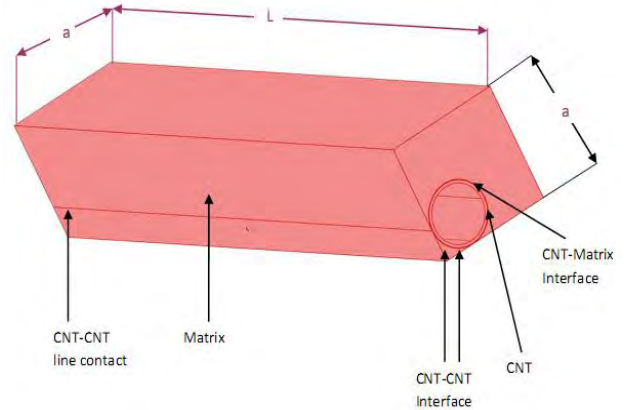


Figure 2. RVE for long CNT bundle based composite

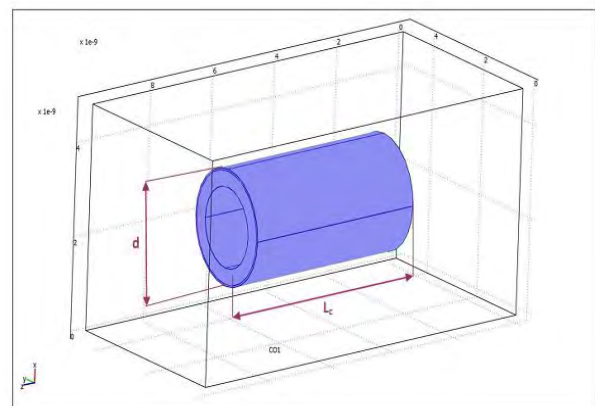
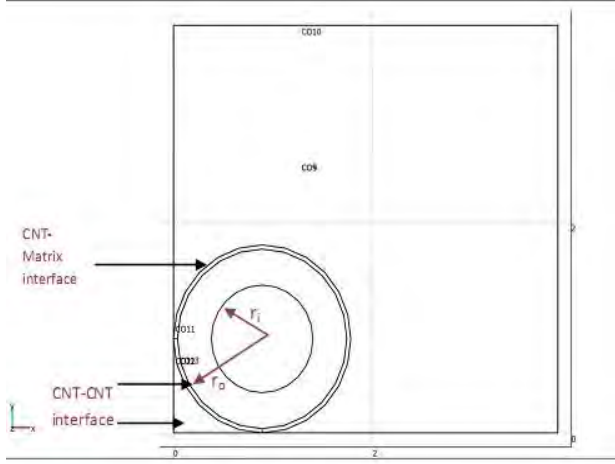


Figure 3. RVE for short single CNT based composite (inside view)



**Figure 4.** Cross sectional view of the RVE for short CNT bundle based composite

### 2.1 Calculation of CNT Radius:

The value of the chiral indices (m,n) are put in the Eq. (1) and we can get the value of mean radius of the CNT. Then using Eq. (2) we can get the outer radius ( $r_o$ ) and inner radius ( $r_i$ ). The chiral indices taken into account here are (10,10); (15,15); (20,20) for both long and short CNT.

$$r_{\text{mean}} = \frac{\sqrt{3} \times 0.1444 \times \sqrt{(m^2 + m^2 + mn)}}{2\pi} \quad (1)$$

$$r_o - r_i = 0.34 \quad (2)$$

$$r_o = r_{\text{mean}} + 0.17 \quad (3)$$

$$r_i = r_{\text{mean}} - 0.17 \quad (4)$$

### 2.2 Volume Fraction of Long CNT in CNT-Matrix Composite

In case of long CNT based composite, the CNT is relatively long (with large aspect ratio) and it is through out the RVE. For the square RVE, the volume fraction of the CNT (a tube) (Fig.1) is defined by the following equation.

$$V^l = \frac{A_f L}{A_c L}$$

$$V^l = \frac{\pi (r_o^2 - r_i^2)}{a^2 - \pi r_i^2} \quad (5)$$

In this paper the volume fraction is always kept 5%. So in Eq. (5) we put the value of  $r_o, r_i$  (from previous calculation) and volume fraction and thus get the value of the width (a) of the square RVE.

### 2.3 Volume Fraction of Short CNT in CNT-Matrix Composite

In case of short CNT based composite, the CNT is embedded inside the RVE. For the square RVE, the volume fraction of the CNT (a tube) (Figure 3.) is defined by the following equation.

$$V^t = \frac{A_f L_c}{(A_c L_c + a^2 L_e)} \quad (6)$$

$$\text{Where, } A_f = \pi(r_o^2 - r_i^2)$$

$$\text{And } L = L_c + L_e$$

$r_o$	CNT outer radius
$r_i$	CNT inner radius
$L$	Length of the RVE
$L_c$	Length of the CNT

### 2.4 Rule of Mixtures Based on the Strength of Materials Theory

For the validation we evaluated both the longitudinal and transverse Young's modulus. The effective Young's modulus  $E_z$  for long CNT based composite in the axial direction is found to be-

$$E_z = E^t V^t + E^m (1 - V^t) \quad (7)$$

The effective Young's modulus  $E_z$  for short CNT based composite is found to be

$$E_z = \frac{1}{\frac{1}{E^m} \times \left(\frac{L_c}{L}\right) + \frac{1}{E^t} \times \frac{L_c}{L} \times \frac{A}{A_c}} \quad (8)$$

The Transverse Young's modulus  $E_x$  for long CNT based composite is found to be

$$E_x = \frac{1}{\frac{V^t}{E^t} + \frac{V^m}{E^m}} \quad (9)$$

### 3. Interface Properties

Among the many factors that govern the characteristics of composites involving a fibrous material it is certain that the adhesion between fiber and matrix plays a predominant part. The stress transfer at the interface requires an efficient coupling between fiber and matrix. It is important to optimize the interfacial bonding since a direct linkage between fiber and matrix gives rise to a rigid, low impact resistance material. Nanocomposites possess a large amount of interfaces due to the small size (nanometer) of reinforcements. The interface behavior can significantly affect the mechanical properties of nanocomposites, since load from the matrix to the fibers is transferred through this interface. The interface between CNT-matrix is considered to be 0.04 nm thickness. But the interface between CNT-CNT is varied according to the diameter of the CNTs.

**Table 1.** Properties Of CNT, Matrix, CNT-CNT interface, CNT-Matrix interface taken into account in this paper

	CNT	Matrix	CNT-Matrix Interface (with only vdW interaction)	CNT-CNT Interface (with only vdW interaction)
Young's Modulus, E	1 TPa	5 GPa	2.7 MPa	5.35 MPa
Poisson's Ratio, $\nu$	0.3	0.3	0.3	0.3

### 4. COMSOL Multiphysics 3.5

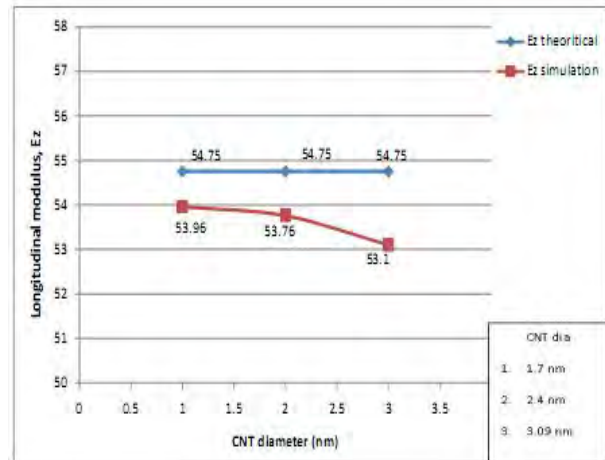
After getting all the values of CNT outer radius, CNT inner radius, width and length of square of the matrix and thickness of interface the model is made. After setting all the boundary conditions, the whole structure is meshed. Then the problem is solved and all the results are obtained from postprocessing options. All these works are done by COMSOL Multiphysics 3.5

### 5. Results and Discussions

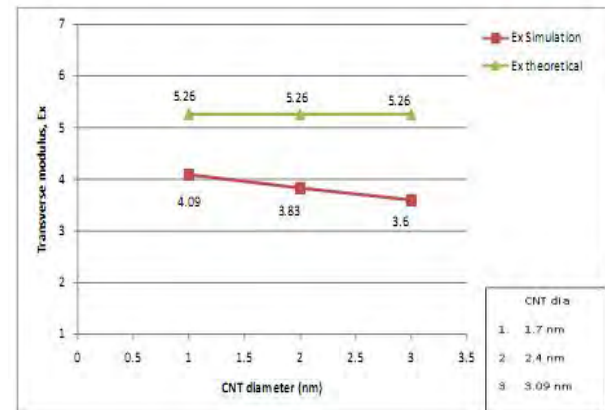
First of all validations of the models are done and then the effects of bundle diameter and length of CNTs' on CNT reinforced polymer are discussed.

#### 5.1 Validation for Long Single CNT Based Composite

To validate the present finite element model for single CNT based composite, FEM results are compared with those of 'Rule of Mixtures'. In this paper the model has an interface but 'Rule of Mixtures' has no consideration of interface.



**Figure 5.** Ez versus CNT diameter graph for long single CNT based composite

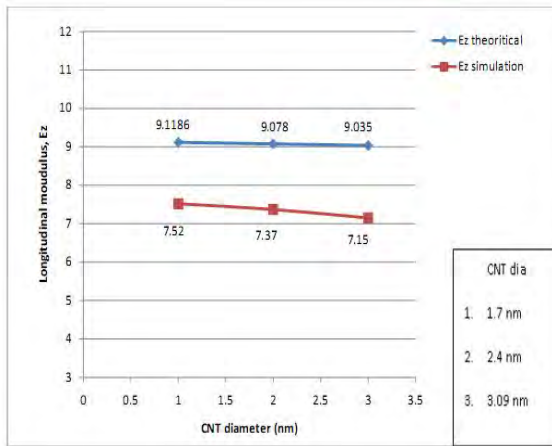


**Figure 6.** Ex versus CNT diameter graph for long single CNT based composite

From Figure 5, it is observed that the theoretical values of Longitudinal Young's modulus remain 54.75 GPa for any CNT diameter. But the values which is obtained from simulation varies from 53.96 to 53.1 GPa. Again from Figure 6, it is observed that the theoretical values of Transverse Young's modulus remain 5.26 GPa for any CNT diameter. But the values which is obtained from simulation varies from 4.09 to 3.6 GPa. So there is little difference between theoretical and simulation values. This is because in simulation the effect of interface is considered whereas in theoretical case there is no consideration of interface. So the validation of the models of long single CNT based composite is done.

### 5.2 Validation for Short Single CNT Based Composite

To validate the present finite element model for single CNT based composite, FEM results are compared with those obtained from Eq.(8). In this eq. the effect of interface is not taken into account whereas in the model there is interface.



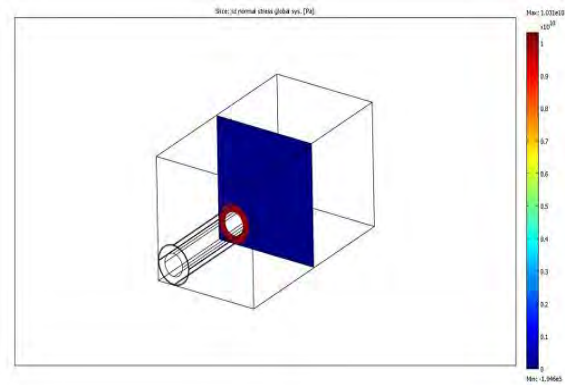
**Figure 7.** Ez versus CNT diameter for short single CNT based composite

From Figure 7, it is observed that the theoretical values of Longitudinal Young's modulus remain between 9.1186 to 9.035 GPa for CNT diameter of 1 to 3 nm. But the values which is obtained from simulation varies from 7.52 to 7.15 GPa. So there is little difference between theoretical and simulation values. This is because in

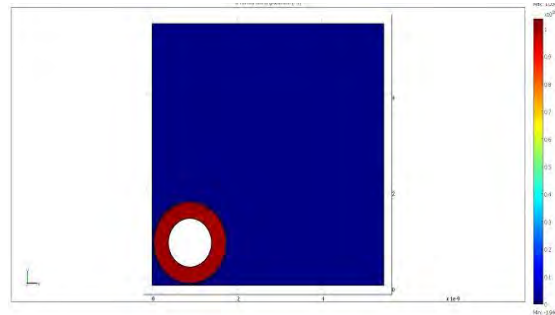
simulation the effect of interface is considered whereas in theoretical case there is no consideration of interface. So the validation of the models of short single CNT based composite is done.

### 5.3 Effects of Bundle Diameter on Composite Elastic Properties

The volume fraction of CNT is kept 5% in all the analysis. The CNT chiral indices (10, 10), (15, 15) and (20, 20) are considered for diameter effect determination. A cross section is taken along the width of the model to calculate the value of longitudinal Young's modulus.



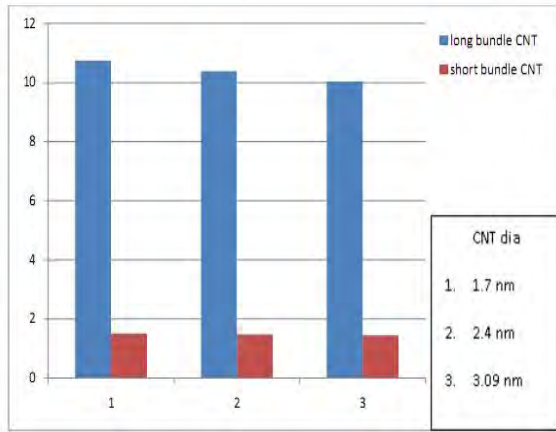
**Figure 8.** Plot of longitudinal stress for long bundle CNT based composite.



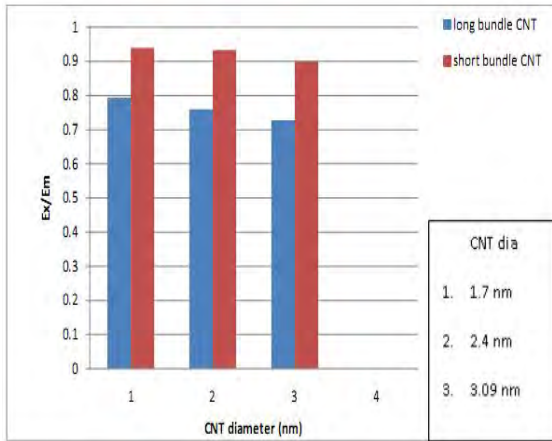
**Figure 9.** Plot of longitudinal stress on the cut-plane.

In Figure 9, we can see the stress distribution in the cross section plane. The stress concentration is much higher in CNT than the matrix.

In case of calculating transverse Young's modulus the cross section is taken along the length of the model



**Figure 10.**  $E_z/E_m$  versus CNT diameter for CNT bundle based composite



**Figure 11.**  $E_x/E_m$  versus CNT diameter for CNT bundle composite

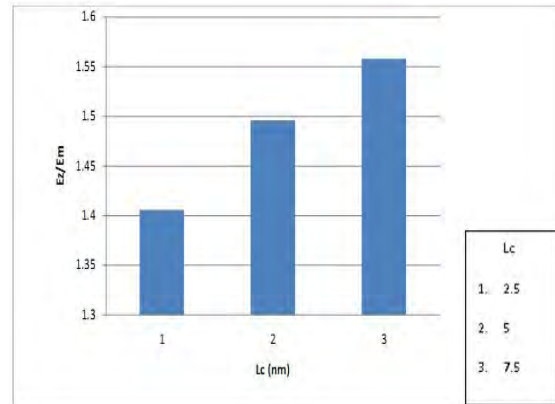
From Figure 10. we see that as the CNT diameter increases from 1.7 nm to 3.09 nm, the longitudinal Young's modulus ratio ( $E_z/E_m$ ) for long bundle based CNT composite decreases from 10.74 to 10.04. From Figure 11. we see that as the CNT diameter increases from 1.7 nm to 3.09 nm, the transverse Young's modulus ratio ( $E_x/E_m$ ) for long bundle based CNT composite decreases from 0.78 to 0.72.

From Figure 10. we see that as the CNT diameter increases from 1.7 nm to 3.09 nm, the longitudinal Young's modulus ratio ( $E_z/E_m$ ) for short bundle based CNT composite decreases from 1.58 to 1.45. From Figure 11. we see that as the CNT diameter increases from 1.7 nm to 3.09

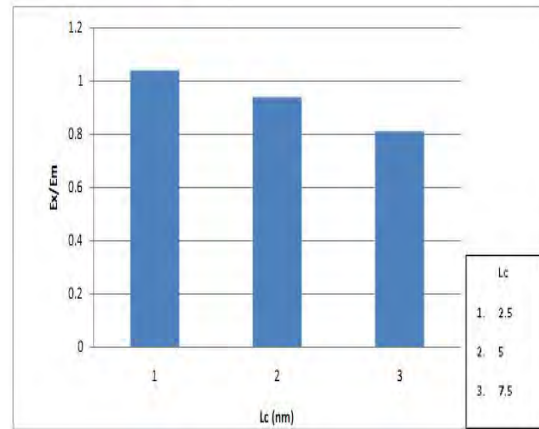
nm, the transverse Young's modulus ratio ( $E_x/E_m$ ) for short bundle based CNT composite decreases from 0.94 to 0.90.

#### 5.4 Effects of Fiber Length on Composite Elastic Properties

The volume fraction of CNT is kept 5% and diameter of the CNT is considered 0.85 nm in all the analysis. In case of short CNT consideration the CNT length ( $L_c$ ) of 2.5 nm, 5 nm and 7.5 nm are considered for length effect determination.



**Figure 12.**  $E_z/E_m$  versus fiber length for short CNT bundle based composite



**Figure 13.**  $E_x/E_m$  versus fiber length for short CNT bundle based composite

From Figure 12. we see that as the CNT length increases from 2.5 nm to 7.5 nm, the longitudinal Young's modulus ratio ( $E_z/E_m$ ) for short CNT bundle based CNT composite

increases from 1.406 to 1.558. From Figure 13, we see that as the CNT length increases from 2.5 nm to 7.5 nm, the transverse Young's modulus ratio ( $E_x/E_m$ ) for short bundle based CNT composite decreases from 1.02 to 0.81.

## 6. Conclusion

The conclusion can be summarized as:

- Validation for single CNT is done by making a model with interface. This is done by evaluating the Young's Modulus from simulation and comparing with that of 'Rule of mixtures'. There is some difference because of the consideration of interface in simulation.
- Change of long CNT bundle diameter affects the composite Young's Modulus. With the increase of CNT bundle diameter the longitudinal Young's modulus and transverse Young's modulus of the composite decreases.
- Change of short CNT bundle diameter affects the composite Young's Modulus. With the increase of CNT bundle diameter the longitudinal Young's modulus and transverse Young's modulus of the composite decreases.
- Change of CNT bundle length has significant effects on the composite Young's Modulus. The Young's Modulus of short CNT bundle based composite increases in longitudinal direction with the increase of CNT bundle length. However, in the transverse direction, Young's Modulus decreases with the increase of CNT bundle length.

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