Influence of Matrix Stiffness, CNT Thickness, Poisson's Ratio, and Interphase on Effective Longitudinal Modulus of CNT Based Composites for Square RVE

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Md. Mohiuddin[1] Mohammad Abu Hasan Khondoker[2] Golam Kabir[3] Md. Abdulla Al Masud[4]

***Abstract*-This paper presents a computational modeling approach for evaluating the mechanical behavior of CNT based nanocomposite. The CNT's interaction with matrix material was modeled using the continuum mechanics theory and finite element approach. The effective mechanical properties of CNT based nanocomposite were then evaluated by using the finite element method (FEM) models. Two different models were constructed. The first model was a CNT through the length of the square representative volume element (RVE). The second model considers a CNT inside the square representative volume element (RVE). Several numerical examples were carried out to investigate the influence of Young's modulus of matrix, CNT thickness, Poisson's ratio and interphase on the effective modulus of CNT based nanocomposite in longitudinal direction. The computed results were compared with those obtained from the simple rule of mixture for validity.**

Keywords-Carbon nanotube, Finite element method, Representative volume element

I. Introduction

Simulations of individual CNTs using atomistic or molecular dynamics (MD) models have provided abundant results for the understanding of mechanical and electrical behaviors of the CNTs (Kang and Hwang, 2001; Garg and Sinnott, 1998). However, these atomistic or MD simulations are currently limited to very small length and time scales and cannot deal with the larger length scales in nanocomposites, due to the limitations of current computing power (for example, a 1 × 1 × 1 μm3 cube could contain up to 1012 atoms). Nanocomposites for engineering applications expand from nano to micro, and eventually to macro length scales, which must be addressed by other simulation approaches or combinations of MD with other approaches. Continuum approaches based on continuum mechanics have also been applied successfully for simulating the mechanical responses of individual or isolated carbon nanotubes which are treated as beams, thin shells or solids in cylindrical shapes (Govindjee and Sackman, 1999). These studies suggest that the continuum mechanics approach can be applied safely to investigate the mechanical behaviors of the CNTs when the lengths of the CNTs are about 100 nm and above. For example, in the study of Wong et al., 1997, the authors successfully applied the simple beam theory to model CNTs and extracted Youngs modulus of the CNT from the force–deflection curve obtained from their experiment. Their results are consistent with other reported work. Although successful to some extent and efficient in computation for models at larger length scales, continuum mechanics at this threshold faces the risk of breakdowns more than ever before, compared with the micromechanics simulations. The preferred approach for simulations of CNT-based composites should be a multiscale one where the MD and continuum mechanics are integrated in a computing environment that is detailed enough to account for the physics at nanoscales while efficient enough to handle nanocomposites at larger length scales. Before a multiscale approach for simulations of nanocomposites is successfully developed, the continuum mechanics approach seems to be the only feasible approach now for conducting some preliminary studies of such materials.

Nomenclature:

ε_z = longitudinal extension resulting from the load in the composite

ε_z^t = longitudinal extension resulting from the load in the CNT

ε_z^t = longitudinal extension resulting from the load in the matrix

E^t = Young's modulus of the CNT

E^m = Young's modulus of the matrix

V^t = Volume fraction of the CNT = $(1-V^m)$

V^m = Volume fraction of the matrix = $(1- V^t)$

V = Volume of the total composite

A^t = Cross-sectional area of the CNT

A^m = Cross-sectional area of the matrix

A = Cross-sectional area of the total composite

F_z = Total force applied at longitudinal direction

F_t = Force shared by only CNT

F_m = Force shared by only matrix

σ_z = Total stress applied at longitudinal direction

σ_t = Stress experienced by only CNT

σ_m = Stress experienced by only matrix

About-[1]Department of Industrial and Production Engineering, Bangladesh University of Engineering and Technology, Bangladesh
About-[2]Department of Industrial and Production Engineering, Bangladesh University of Engineering and Technology, Bangladesh
About-[3]Department of Industrial and Production Engineering, Bangladesh University of Engineering and Technology, Bangladesh
About-[4]Department of Industrial and Production Engineering, Bangladesh University of Engineering and Technology, Bangladesh
(e-mail: aamasud@ipe.buet.ac.bd)

r_i = Inner radius of CNT
r_o = Outer radius of CNT
a = Side of the matrix of square RVE

In the study of Liu and Chen, 2002 the interactions of the CNT with the matrix, interfacial stresses and load-carrying capabilities of the CNTs are investigated based on 3-D elasticity models. It is proposed in that instead of beam or shell models, the 3-D elasticity models should be used for the CNTs, as well as the matrix, in order to ensure the accuracy and compatibility of the models for the CNTs and the matrix (Liu and Chen, 2002). One way to develop manageable 3-D continuum models for the study of CNT-based composites is to extend the concept of representative volume elements used for conventional fiber-reinforced composites at the microscale (Nasser and Hori, 1999). CNTs are in different sizes and forms when they are dispersed in a matrix to make a nanocomposite. They can be single-walled or multi-walled with length of a few nanometers or a few micrometers, and can be straight, twisted and curled, or in the form of ropes (Wagner, 2002; Qian et al., 2002). Their distribution and orientation in the matrix can be uniform and unidirectional (which may be the ultimate goal) or random. All these factors make the simulations of CNT-based composites extremely difficult. To start with, the concept of unit cells or representative volume elements, which have been applied successfully in the studies of conventional fiber-reinforced composites at the microscale (Nasser and Hori, 1999) can be extended to study the CNT-based composites at the nanoscale. In this RVE approach, a single (or multiple) nanotube(s) with surrounding matrix material can be modeled, with properly applied boundary and interface conditions to account for the effects of the surrounding materials. Numerical methods, such as the FEM, boundary element method (Liu and Chen, 2002) or meshfree method (Qian et al., 2002) can be applied to analyze the mechanical responses of these RVEs under different loading conditions. Interfaces between the CNTs and matrix are crucial regions to ensure the load carrying capacity and other functionalities of the nanocomposites. There are also more difficult regions for any simulation approaches. To start with, perfect bonding can be assumed between the CNTs and matrix in the continuum mechanics models of CNT-based composites. Research has demonstrated that the possibility of such a strong (C–C) bond exists for CNT-based composites (Thostenson et al., 2005). For a ‗less" perfect bond, a spring-like model can be used between the CNTs and matrix. A thin interphase model (e.g., a thin coating on the CNTs) can also be introduced to account for a third phase between the CNTs and matrix. The properties of this interphase region can be used to characterize the interface properties. Other interface models, such as friction models considering the slip/stick along a CNT/ matrix interface or a van der Waals type of models (Qian et al., 2002) (for multi-walled CNTs) can certainly be developed for modeling CNT-based composites, with improved understanding based on further nanoscale experiments and MD simulations. In this paper, only the perfect bonding between the CNT and the matrix in RVE models is considered. Three nanoscale representative volume elements based on the 3-D elasticity theory have been proposed in Liu and Chen, 2002 for the study of CNT-based composites. They are the cylindrical RVE, square RVE and hexagonal RVE. The cylindrical RVE can be applied to model the CNTs which have different diameters (Riddick and Hyer, 1998) or CNTs embedded in a regular carbon fiber. Under axi-symmetric as well as anti-symmetric loading, a 2-D axi-symmetric model can be applied for the cylindrical RVE, which can significantly reduce the computational work (Govindjee and Sackman, 1999). Similar to the study of conventional fiber-reinforced composites (Riddick and Hyer, 1998) the square RVE models can be applied when the CNTs are arranged evenly in a square array, while the hexagonal RVE models can be applied when CNTs are in a hexagonal array, in the transverse direction. These RVEs can be used to study the interactions of a CNT with the matrix, such as the load transfer mechanism and stress distributions along the interfaces (Govindjee and Sackman, 1999) or to evaluate the effective material properties of the CNT-based composites, which is the focus of this current paper.

To start with, the cylindrical RVE will be employed first in this paper to evaluate the effective Young‘s moduli and Poisson‘s ratios of the CNT based composites. The required mathematical results to be used to extract these material constants from the simulation results (by using either the FEM or other methods) will be established in section 2. In section three finite elements modeling technique for long continuous and short fiber is described. In results and discussion section, influence of matrix young modulus, CNT thickness, Poisson‘s ratio and interphase on the longitudinal elastic modulus of CNT based composites is studied.

II. Analysis

Depending on the problem definition, geometry, boundary conditions and material properties, three types of analysis can be performed on a structure. 2D analysis is mainly used to conserve the computational resources. It is less time consuming and is less accurate. 3D analysis is time consuming approach requiring high computational resources because of the 3-D elements used. It is relatively accurate than 2D analysis, and is used in situations where 2D degeneration is not possible. Symmetric analysis is performed taking advantage of the symmetric geometry. A quarter or half the model is created and analyzed by applying symmetric boundary conditions. This approach significantly reduces the cost, computer memory and the time required. In this study symmetric analysis is performed for the RVE models by modeling only the quarter model of the geometry and applying axi-symmetric boundary conditions.

Computational approaches consists of both molecular dynamics approach and numerical or continuum mechanics. Continuum mechanics in the past has been successfully used in characterizing CNT based composites. It is a very feasible, cost effective and an efficient approach at present to characterize large-scale CNT-based composites for mechanical properties using the finite element modeling and simulations. Preliminary results obtained in this research can be compared with the available experimental and MD results from similar models reported in previous literature (Treacy et al., 1996). In all the studies performed in the literature (Thaw et al., C., 1987; Mortensen et al., 1988), CNTs are considered as homogeneous and isotropic materials and are represented by continuum beam, shell and 3-D solid elements. This approach is in general used to analyze for deformation, buckling, and dynamic responses of CNTs and overall response of the nanocomposite. Using this approach, emphasis is to be placed on overall responses of the CNT based composites and load carrying capabilities rather than the localized detailed phenomena, like interfacial stresses or bonding. MD approach, on the other hand, is preferred in studying the detailed interfacial characteristics.

Continuum mechanics approaches like the BEM other than the FEM are turning out to be ideal tools for RVE model, nanocomposites, and its validation has been demonstrated in previous literature (Gao et al., 1998; Buongiorno et al., 2000). This concept has been successfully applied in the past for characterizing conventional fiber-reinforced composites. The same has been extended to nanocomposites here. This kind of model works by modeling a single CNT or multiple CNTs in a surrounded matrix with appropriate boundary conditions and interface conditions (perfect bonding assumed in our case). Later on, after modeling the RVE model the FEM is applied to characterize for the overall mechanical response of the RVE (effective Young‘s modulus of the composite). Modeling considerations in characterizing CNT-based composites have been proposed and discussed in (Thaw et al., C., 1987). The first and foremost task is to employ 3-D elasticity models replacing beams and shell models for modeling CNT-based composites. This is basically to ensure accuracy and compatibility between CNTs and matrix in the composite. Hence 3-D solid elements for both CNTs and matrix have been used in the models demonstrated by Liu and Chen (2004) in characterizing CNT-based composites. The results reported are in complete agreement with the rule of mixtures results, although further development and validation of their models was required. The research work performed here successfully validates the FEM results with MD, constitutive modeling and rule of mixtures as well. The validation and agreement of the continuum mechanics results can play a significant role for numerical approaches like the FEM, which can be further used for characterizing large models. Emphasis is being placed on modeling large-scale composite models using pipe elements instead of beam and shell elements. The results shown in section 4 challenges that FEM can be an excellent estimate for evaluating elastic moduli of large-scale composites. Hence FEM, which is cost effective and efficient, in the future can be used for characterizing nanocomposites, significantly reducing computational time, memory and hard-disk space.

In this experiment it is assumed that both the CNTs and matrix in a RVE are continua of linearly elastic, isotropic and homogenous materials, with given Young‘s moduli and Poissons ratios. It is also assumed that the CNTs and matrix are perfectly bonded at the interface in the RVE to be studied. Other material models and interface conditions (Chen and Liu, 2002) can certainly be considered in more sophisticated investigations. The RVE can contain one CNT or multiple CNTs, determined by the main criterion that it should be large enough to be representative of the material and small enough to be modeled and analyzed efficiently using a solution method. Under the above assumptions, there will be four effective material constants to be determined for the CNT-based composite, namely, two Young‘s moduli E_x (= E_y) and E_z, and two Poisson‘s ratios ν_{xy} and ν_{zx} (= ν_{zy}). To derive the formulas for extracting the four material constants, a homogenized elasticity model corresponding to the RVE is considered. The geometry of the elasticity model is corresponding to a hollow cylindrical RVE with length L, inner radius r_i and outer radius R, so that analytical solutions can be obtained. This geometry can account for the cases when the CNT is relatively long and thus all the way through the length of the RVE. In the case that the CNT is relatively short and thus fully inside the RVE, a solid cylindrical RVE (r_i = 0) can be used for extracting the material constants, since the elasticity solutions are difficult to find in this case. The elasticity model has a single material with the four effective material constants (E_x, E_z, ν_{xy} and ν_{zx}) to be determined.

The geometry of the elasticity model is corresponding to a hollow cylindrical RVE with length L, inner radius r_i and outer radius R. This geometry can account for the cases when the CNT is relatively long and thus all the way through the length of the RVE. In the case that the CNT is relatively short and thus fully inside the RVE, a solid cylindrical RVE (r_i = 0) can be used for extracting the material constant, since the elasticity solution are difficult to find in this case.[12]

For axial loading, the stress and strain components at any point on the lateral surface are,

$\sigma_r = \sigma_\theta = 0$

$\varepsilon_z = \dfrac{\Delta L}{L}$ And $\varepsilon_\theta = \dfrac{\Delta R_a}{R}$

With $\Delta Ra < 0$, if $\Delta L > 0$. Where ΔRa is the radial displacement and r and θ indicate the radial and tangential components respectively. So,

$$\varepsilon_z = \frac{\sigma_z}{E} - \nu\frac{\sigma_z}{E} - \nu\frac{\sigma_\theta}{E}$$

$$\text{Then, } E_z = \frac{\sigma_z}{\varepsilon_z} = \frac{\Delta L}{L}\sigma_{avg} \quad (1)$$

Where the averaged stress is given by

$$\sigma_{avg} = \frac{1}{A}\iint_A \sigma_z\left(x, y, \frac{L}{2}\right) dx\, dy \quad (2)$$

Where, A is the area of the end surface and σ_{avg} can be found for the RVE using the FEM results (i.e.) from the ANSYS 10.0 outputs. Thus, to evaluate the effective Young‘s modulus of the CNT based nanocomposites; the RVEs are studied using the finite element method first. Then the deformations and stresses are computed for the axial loading case. After that, the FEM results are processed and equations are used to extract the effective Young‘s modulus for the CNT based composites.

A. Rule of Mixtures Theory for Long CNT

Prediction of effective material properties of the compositebased on strength of materials theory is given by simpleanalytical expressions (rule of mixtures). This rule ofmixtures along with some extended results in the case of fiber-reinforced composites has been successfully applied in the past for carbon nanocomposites. The effective longitudinal Young‘s modulus of the CNT–reinforced composite using the rule of mixtures expression is used here to validate the numerical results obtained using the FEM. However this strength of materials theory is not accurate when evaluating the interfacial stress but is found to be efficient and accurate in predicting the effective material constants (Young‘s modulus, Poisson‘s ratio) in the axial and transverse direction of the RVE‘s, which are dependent on the overall responses of the RVE‘s.

The addition of long or continuous CNTs (with large aspect ratio i.e., the ratio of the characteristic length L to the characteristic diameter D of the CNT) to a polymer matrix mainly enhances its stiffness and strength. Taking advantage of the continuous structure only a segment can be modeled using RVE, which is shown in Figure 1.

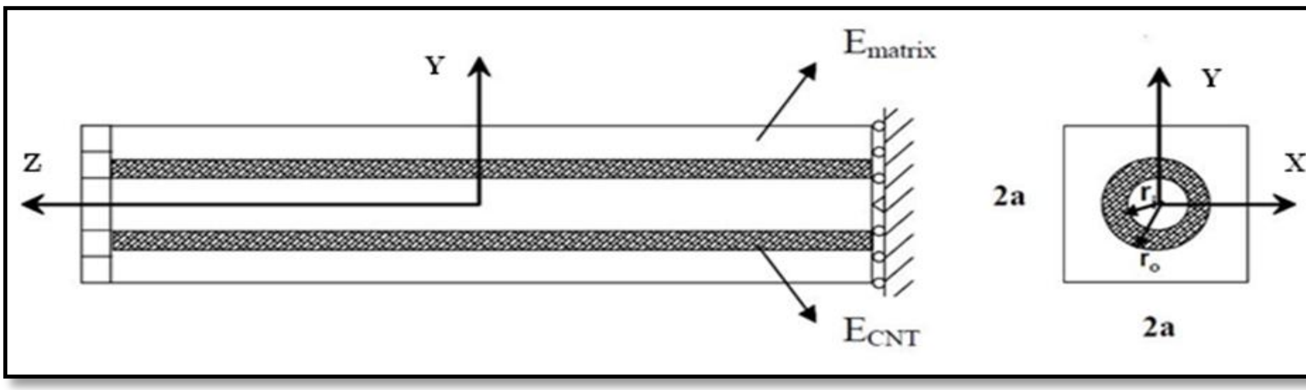

Figure 1: Continuous Fiber Reinforced Inside the Matrix

Therefore, a segment can be modeled using an RVE under some assumptions. They are-

1. CNT fibers are uniform, parallel and continuous
2. Perfect bonding between CNT and matrix therefore, load applied is shared by both CNT and matrix. So,

$$F_z = F_t + F_m$$

3. Longitudinal load produces equal strain in CNT and matrix: It is assumed that the longitudinal extensions resulting from the load are the same in the composite, CNT and the matrix. So,

$$\varepsilon_z = \varepsilon_z^{\,t} = \varepsilon_z^{\,t}$$

Stress can be calculated from force divided by area experiencing the stress. So,

$$\sigma_z A = \sigma_t A^t + \sigma_m A^m \qquad (3)$$

Now, according to Hooke‘s law, Young‘s modulus is the ratio of stress by strain. So,

$$E_z\, \varepsilon_z A = E^t \varepsilon_z^{\,t} A_t + E^m \varepsilon_z^{\,t} A_m$$

Then, $E_z A = E^t A^t + E^m A^m$

And, $E_z = E^t \left(\frac{A^t}{A}\right) + E_m \left(\frac{A^m}{A}\right)$

Finally, $E_z = E^t V^t + E^m V^m = E^t V^t + E^m (1-V^t)$ (4)

For a square RVE the volume fraction of the CNT is defined by

$$V^t = \frac{\pi({r_o}^2 - {r_i}^2)}{(4a^2 - \pi\, {r_i}^2)} \qquad (5)$$

This is the same rule of mixtures, which is being applied for predicting the effective Young‘s modulus for the conventional fiber-reinforced composite in the fiber direction. It has been verified in the past for the agreement with the experimental results obtained from carefully controlled experiments for tensile loading. It agrees well (within 5%) while the predictions are not so good for the compressive loading case.

B. Rule Of Mixtures Theory For Short CNT

Short nanotube reinforced composites analyzed in the past, found not as strong as composites with continuous nanotubes and cannot be used for critical structural applications. It has been demonstrated from molecular dynamics (Qian et al., 2003) and continuum mechanics that the effective modulus of the composite using short CNTs is far less compared to the increase in modulus using long (continuous) CNTs. In this case, the RVE can be divided into two segments: one segment accounting for the two ends with total length L_e and Young‘s modulus E_m; and another segment accounting for the center part with length L_c and an effective Young‘s modulus E_C

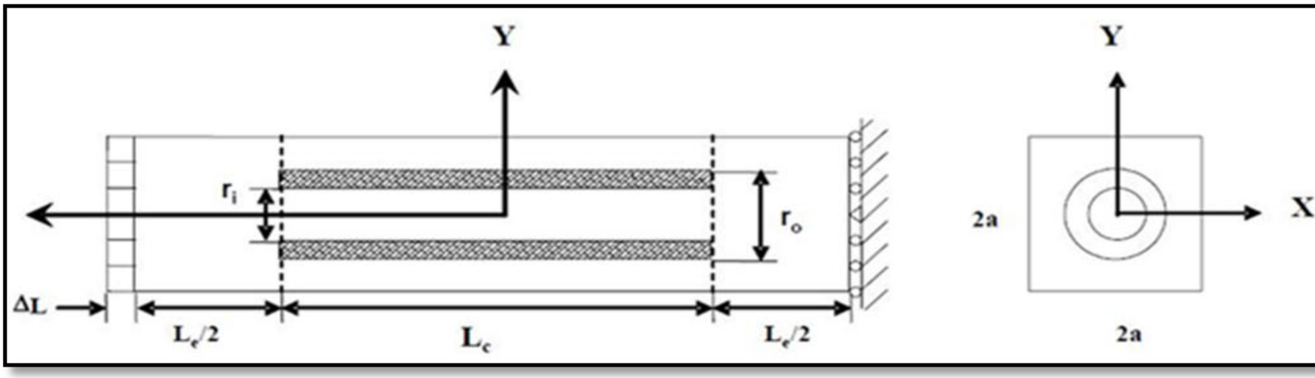

Figure 2: Short Fiber Reinforced Inside the Matrix

It is Notable that the two hemispherical end caps of the CNT have been ignored in this derivation. Since the center part is a special case of long CNT, its effective Young's modulus is found to be

$$E^c = E^t V^t + E^m (1 - V^t) \tag{6}$$

Again, by considering the compatibility of strains and equilibrium of stresses, one obtains the following expression for the effective Young's modulus in the axial direction.

$$E_z = \left[\frac{1}{E^m}\left(\frac{L_e}{L}\right) + \frac{1}{E^c}\left(\frac{L_c}{L}\right)\left(\frac{A}{A_c}\right)\right]^{-1} \tag{7}$$

Alternatively, in a more symmetric form:

$$\frac{1}{E_z} = \left[\frac{1}{E^m}\left(\frac{L_e}{L}\right) + \frac{1}{E^c}\left(\frac{L_c}{L}\right)\left(\frac{A}{A_c}\right)\right] \tag{8}$$

In which the areas $A = 4a^2$ and $A_c = (4a^2 - \pi r_i^2)$, above equation can be viewed as an extended rule of mixtures compared to that given in Equation (1), and can be employed to estimate the effective Young's modulus for the short CNT case when the CNT is inside the RVE. The equation of rule of mixture when using an additional interphase between CNT and matrix

$$E^c = K^1 E^t V^t + K^2 E^I V^I + E^m (1 - V^t - V^I) \tag{9}$$

where V^t and V^I are volume fractions of phases 1 and 2, representing carbon nanotubes and interphase respectively, E^t and E^I are properties of phases 1 and 2, representing carbon nanotubes and carbon fibers, respectively, E^m is property of the polymer matrix, K^1 is the CNT efficiency parameter, which will be assumed equal to 1, K^2 is the interphase efficiency parameter, which is equal to 1 for continuous aligned fibers in the direction of alignment.

III. Modeling

In this paper the cylindrical RVEs (Fig.1, 2) for a single-walled carbon nanotube in a matrix material are modeled using the finite element modeling software ANSYS 10.0. The deformations and stresses are computed for the axial loading cases (Fig. 1, 2). Two cases are studied, one on a RVE with a long CNT and the other on a RVE of the same size but with a short CNT.

A. Model Description for Long CNT

In long CNT, matrix was assumed as square with 20nm side length and the total length of matrix was 100nm and 100nm long CNT through the matrix was also assumed. Values of the dimensions and material constants are chosen for this thesis for illustration purposes only, which are within the wide ranges of those for CNTs reported in the literature (Chen and Liu, 2004; Qian et al., 2003; Wong et al., 1997; Lu, 1997 and Li and Saigal, 2007). Length of CNT and matrix was constant throughout the analysis. Model was symmetric so we took the benefit of symmetricity by taking quarter of model to simulate the results. The volumes comprising the NT and matrix immediately adjacent to it are meshed using 20 node bricks containing midside nodes. This allows element edges to be parabolic in shape, which accurately captures the CNT surface (Bradshaw1 et al., 2004). These higher order elements are also well suited to modeling the high strain gradients that exist close to the NT. The remaining volumes were meshed with 8 node bricks to reduce the number of degrees freedom while still providing sufficient detail to capture the slowly varying strain fields closer to the model exterior (Bradshaw1 et al., 2004).

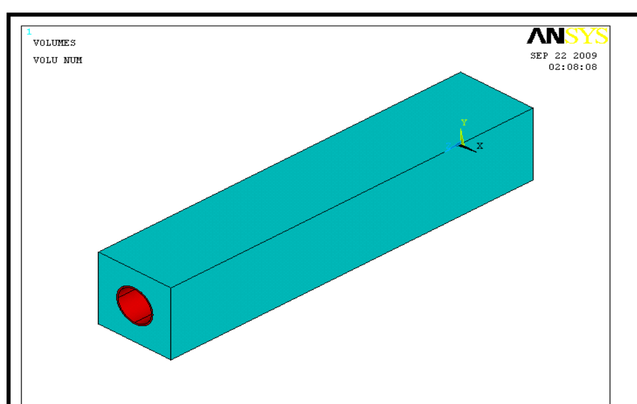

Figure 3: Full Model of Square RVE with Long CNT in Matrix

Proper boundary conditions were applied to the model to find the stress value of the square RVE with long CNT. One end of the matrix and CNT areas was constrained in the axial directions and frees to move in the lateral directions. One of the two free edges was constrained in vertical direction and the other in horizontal direction to allow for the expansion and contraction of the CNT in compression and tension respectively. Symmetric boundary conditions were applied on the quarter model to account for the full model. Displacement boundary conditions instead of pressure boundary conditions were applied on the model to exactly simulate the model as in experimental testing. Pressure boundary conditions on the CNT and matrix makes them elongate with different strain values, with matrix having more elongation than the CNT as CNT has very high stiffness compared to the matrix material. Hence, similar boundary conditions as applied in experimental testing, equal displacements on the matrix and CNT (1nm constant) in the longitudinal direction were applied for analysis, in evaluating the properties of a unidirectional composite (Fisher et al., 2002).

B. Model Description For Short CNT

Like long CNT, matrix of short CNT was assumed as square with 20nm side length and the total length of matrix was 100nm. Short CNT was 50nm in length with 5nm radius of each hemispherical cap. Length of CNT and matrix was constant throughout the analysis. Values of the dimensions and material constants are chosen for this thesis for illustration purposes only, which are within the wide ranges of those for CNTs reported in the literature (Chen and Liu, 2004; Qian et al., 2003; Wong et al., 1997; Lu, 1997 and Li and Saigal, 2007). Model was symmetric so we took the benefit of symmetricity by taking quarter of model to simulate the results[15]. 20 node bricks containing midside nodes used to mesh the CNT and 8 node bricks used to mesh the matrix (Fisher et al., 2002).

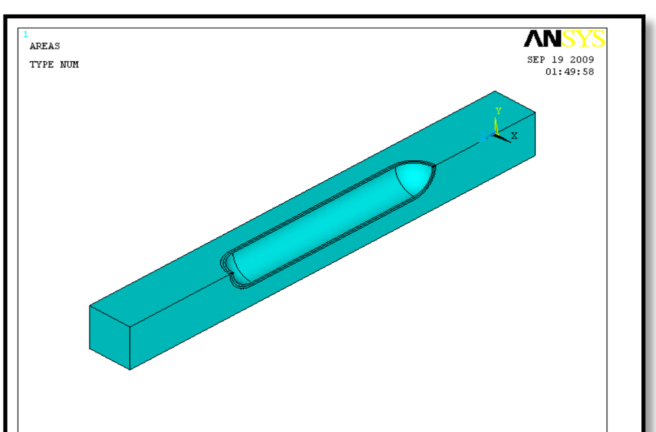

Figure 4: Square RVE, 3D Quarter Model of Short CNT Inside Matrix

Boundary conditions for short CNT-RVE was similar to long CNT model were applied to evaluate the effective longitudinal Young's modulus of the composite. CNT was aligned in axial (loading) direction and the area on one end is totally constrained in axial direction and a displacement of 1nm was applied on the other end. Displacement constraints are so applied that the system was allowed to contract and expand when in tension and compression respectively. Symmetric boundary conditions are applied accordingly to simulate the full model from the quarter model (Chen and Liu, 2004).

IV. Results and Discussion

A. Long Continuous CNT Reinforced RVE

In Long CNT RVE model CNT is through the matrix. In this section effect of matrix stiffness, poisson's ratio, CNT thickness and interphase will be discussed for long fiber. Finite element mesh quarter view of a long continuous CNT based model is shown below.

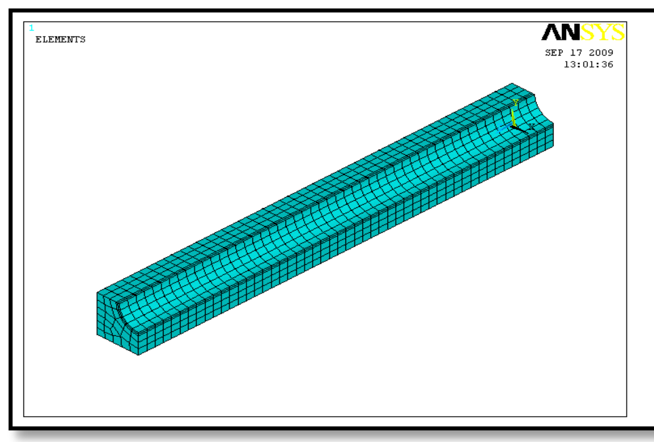

Figure 5: Finite Element Mesh Quarter of Model for the Long CNT Based Model with Et/Em = 1000/30.

B. Effect of Young's Modulus of Elasticity of Matrix on the Effective Longitudinal Modulus of the Nanocomposite (E_z)

Model parameters: For modeling purpose following parameters was used with 0.40nm CNT thickness and 10nm side length according to various previous literatures (Chen and Liu, 2004; Qian et al., 2003; Wong et al., 1997; Lu, 1997; Li and Saigal, 2007 and Bradshaw1 et al., 2004).

Phase	Poisson's ratio	Length (nm)	Young's modulus(GPa)
CNT	0.30	100	1000
Matrix	0.30	100	various

The Effective longitudinal modulus of the Composite is computed at different value of Young's modulus of matrix phase such as 5,10,15,20,25,30,40,50,60,70,80,90,100 using both finite element and rule of mixture. From figure, it was observed that variation of results for FEA and rule of mixture was negligible and effective longitudinal modulus of the Composite increase with the increase of Young's modulus of matrix as which was expected. Changing the value of Young's modulus of matrix from 5 to 100 causes almost 92.4404 GPa increase in effective longitudinal modulus of the nanocomposites. Figure 6 shows below the effective longitudinal modulus of the Composite with the increase of Young's modulus of matrix. Results obtained from rule of mixture theory are also shown in the Figure

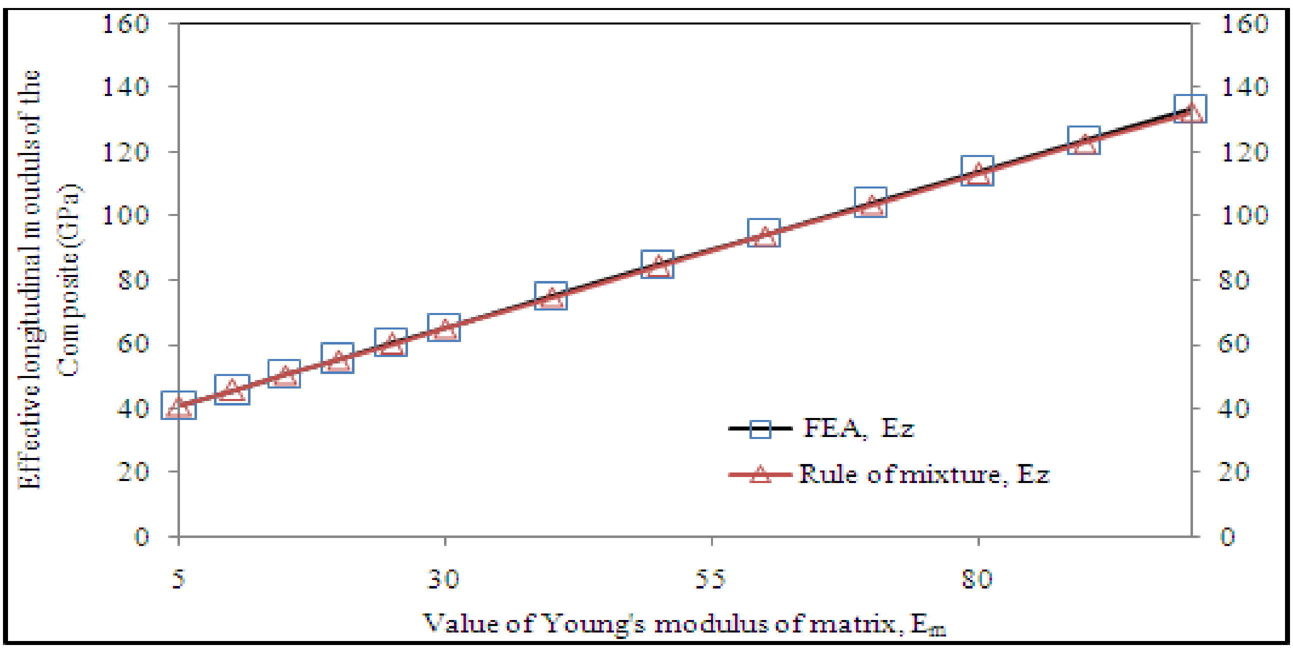

Figure 6: Comparison of Effective Modulus of the Composite in Longitudinal Direction Vs Varying Young's Modulus of the Matrix Reinforced with Long CNT Of Thickness 0.4nm with 3.617% Volume Fraction

C. Effect of Poisson's Ratio on the Effective Longitudinal Modulus of the Nanocomposites

Model parameters: To find the effect of Poisson's Ratio on modulus of nanocomposites following parameters were used according to various previous literatures (Chen and Liu, 2004; Qian et al., 2003; Wong et al., 1997; Lu, 1997; Li and Saigal, 2007 and Bradshaw1 et al., 2004).

Phase	Poisson's ratio	Length (nm)	Young's modulus (GPa)
CNT	Various	100	1000
Matrix	Various	100	30

For all previous simulations the Poisson's ratios of the matrix and nanotube were assumed to be equal (Poisson's ratio of NT=Poisson's ratio of matrix=0.30) to simplify the analysis. For many practical nanotube-polymer systems, the difference in Poisson ratio is expected to be relatively small, with NT typically predicted in the range of 0.20–0.30 and possion' ratio of matrix for a typical structural polymer varies approximately 0.25–0.40 (Fisher et al., 2002). In this paper, Poisson's ratio of matrix and CNT varied from 0.2 to 0.4 to find the effect of various Poisson's ratio in effective longitudinal modulus. Effect of Poisson's ratio on the effective longitudinal modulus of the nanocomposites is Shown in Figure7.

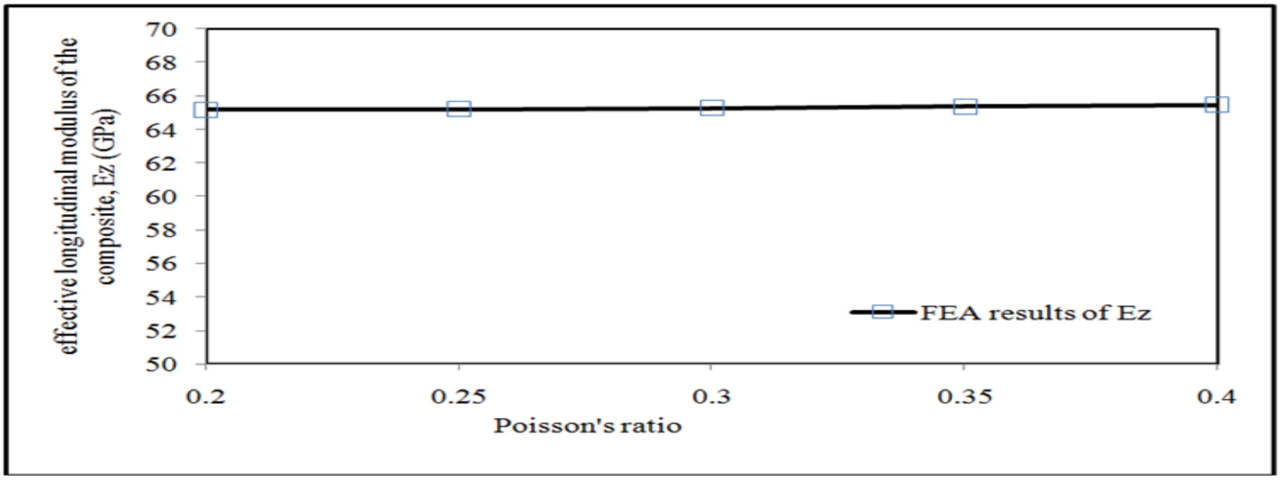

Figure 7: Comparison of Effective Modulus of the Composite in Longitudinal Direction Vs Various CNT and Matrix Poisson's Ratio with Long CNT of Thickness 0.4nm with 3.617% Volume

From the study it is found out that effective longitudinal modulus of the nanocomposites remains same with the increase of both Poisson's ratio of CNT and matrix. With the increase of Poisson's ratio from 0.2 to 0.4, effective longitudinal modulus of nanocomposites increased by 0.4704%. So we found that the effect of the Poisson's ratio of the CNT and matrix on the composite on the simulation is negligible.

D. Effect of CNT Thickness on the Effective Longitudinal Modulus of the Nanocomposites (E_z)

Model parameters

Phase	Poisson's ratio	Length (nm)	Young's modulus(GPa)
CNT	0.30	100	1000
Matrix	0.30	100	30

Composite effective modulus of the composite in longitudinal direction increases with the increase of CNT thickness. It can be explain that as thickness of CNT increase and as usual volume fraction, so total strength of the composite also increases. Because by rule of mixture theory composite's tensile modulus is directly proportional to CNT volume fraction. As CNT's modulus of elasticity is higher than matrix so increases of volume fraction of CNT increases the composite's strength. Figure 8 shows the effect of CNT thickness on the effective longitudinal modulus of the nanocomposites (E_z).

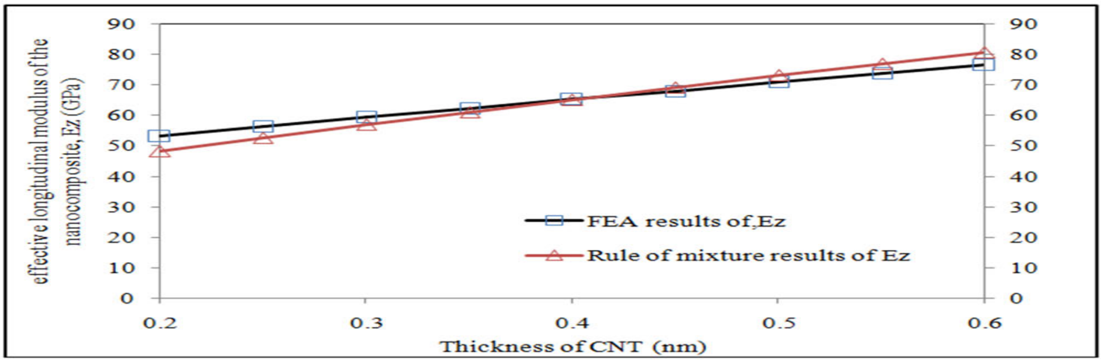

Figure 8: Comparison of Effective Modulus of the Composite in Longitudinal Direction Vs Varying CNT Thickness with Long CNT

CNT volume fraction also increases by increasing the thickness of CNT material without changing the length shown in Figure 9 Actually effective longitudinal modulus of the nanocomposites strongly depends on the volume fraction of CNT material. From the figure and data (thickness of CNT 0.20 with 30 Young's modulus of matrix) we observe that with the addition of only about 1.88% volume fraction of the CNTs in a matrix, the stiffness of the composite in the CNT axial direction can increase as much as 77.087% for the case of long CNT fibers.

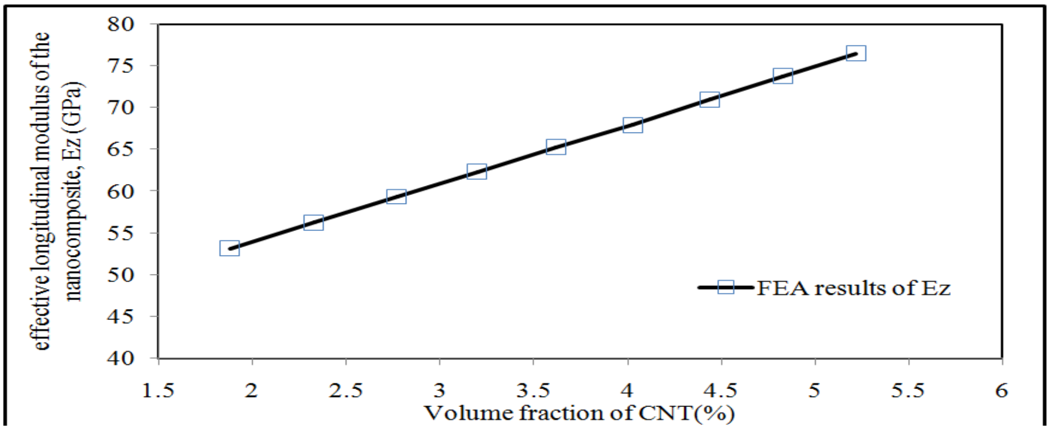

Figure 9: Comparison of Effective Modulus of the Composite in Longitudinal Direction Vs Varying CNT Volume Fraction with Long CNT.

E. Effect of Interphase on the Effective Longitudinal Modulus of the Nanocomposites

The presence of an interphase region between fibers and matrix in a composite system, can significantly affect the load transfer characteristics, even when the interphase is very thin. Three dimensional model of nanocomposite with interphase is shown in Figure 10.

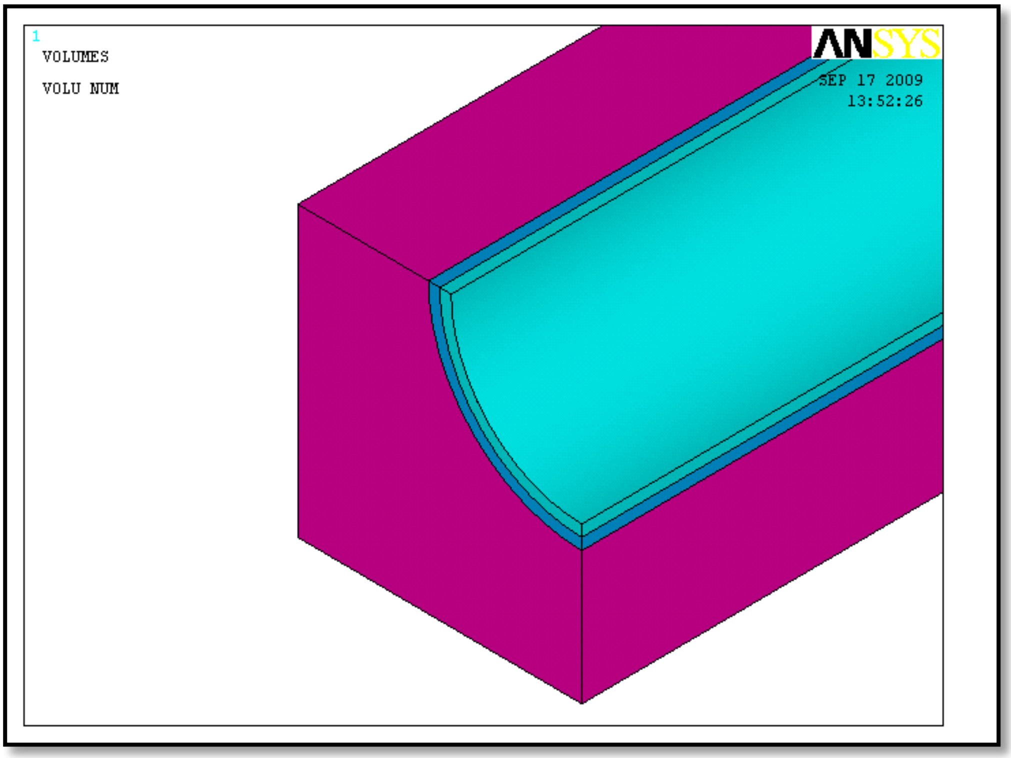

Figure 10: Three Dimensional Close View of Long CNT Nanocomposite with Interphase.

Model parameters

Phase	Poisson‘s ratio	Length (nm)	Young‘s modulus(GPa)
CNT	0.30	100	1000
Matrix	0.30	100	30
Interphase	0.30	100	Variable

For this model we use an interphase of 0.4nm thickness (CNT thickness=0.40nmconstant) and effective longitudinal modulus of the nanocomposite is investigated by changing the Young‘s modulus of interphase shown in Figure 11.

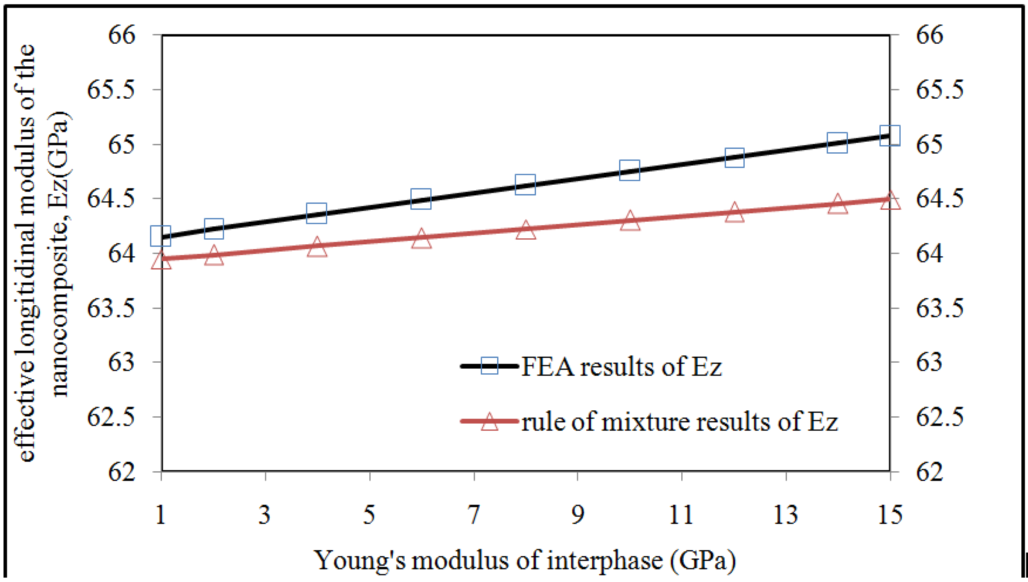

Figure 11: Comparison of Effective Modulus of the Composite in Longitudinal Direction (Both FEA and Rule of Mixture) Vs Varying Young‘s Modulus with Long CNT.

F. Short CNT Reinforced RVE

A short CNT unit cell model is the one in which a CNT short enough compared to long CNT with high D/L ratio and with end caps, is placed in a polymer matrix. It is completely inserted inside the matrix unlike the long CNT model, which is placed from one end to other end in the longitudinal direction in the matrix .From various previous section it is found that short CNTs do not possess good load carrying capabilities and also develop high stress concentrations at the ends of the CNT. First principle stress of short CNT reinforced composites is shown in Figure 12.

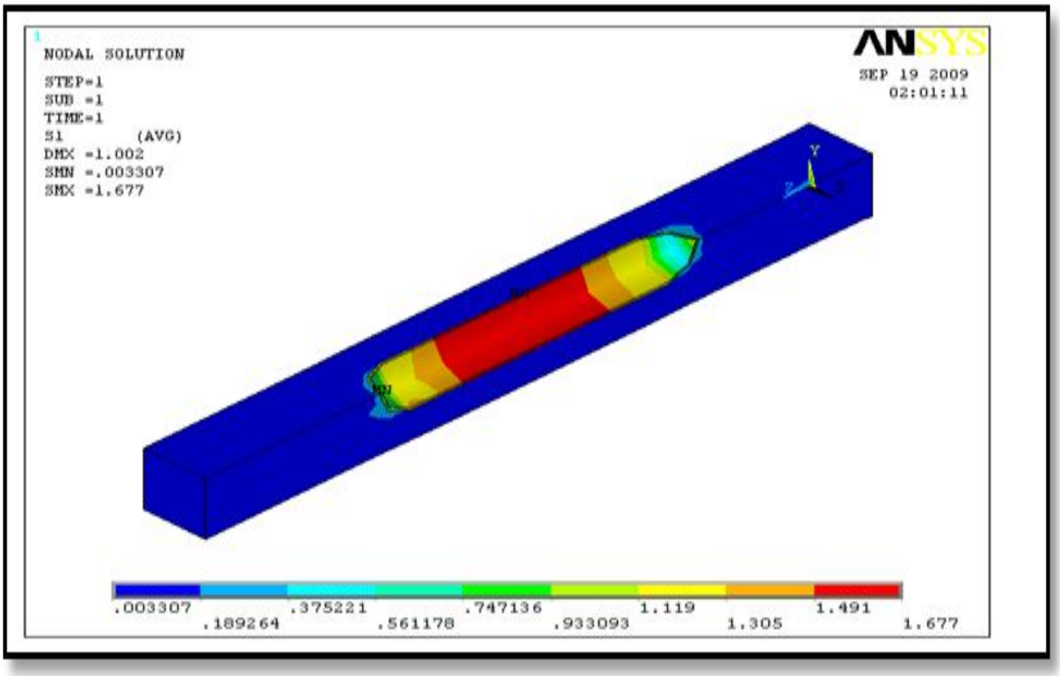

Figure 12: Contour Plot of First Principle Stress of Short CNT-RVE for Matrix Young's Modulus 30gpa and CNT Thickness 0.40nm, Length of CNT 50nm with Side Hemispherical Caps.

G. Effect of Matrix Young's Modulus of Elasticity on the Effective Longitudinal Modulus of the Nanocomposite (E_z) for Short CNT

In this case the model parameters were same as long CNT except the length of CNT is taken as 0.50nm and short CNT is situated at the center of matrix. From Figure 13 we observe that variation of results for FEA and rule of mixture is negligible and Effective longitudinal modulus of the Composite increase with the increase of Young's modulus of matrix which is expected. Changing the value of Young's modulus of matrix from 5 to 100 causes almost 96.5649 GPa increase in effective longitudinal modulus of the nanocomposites.

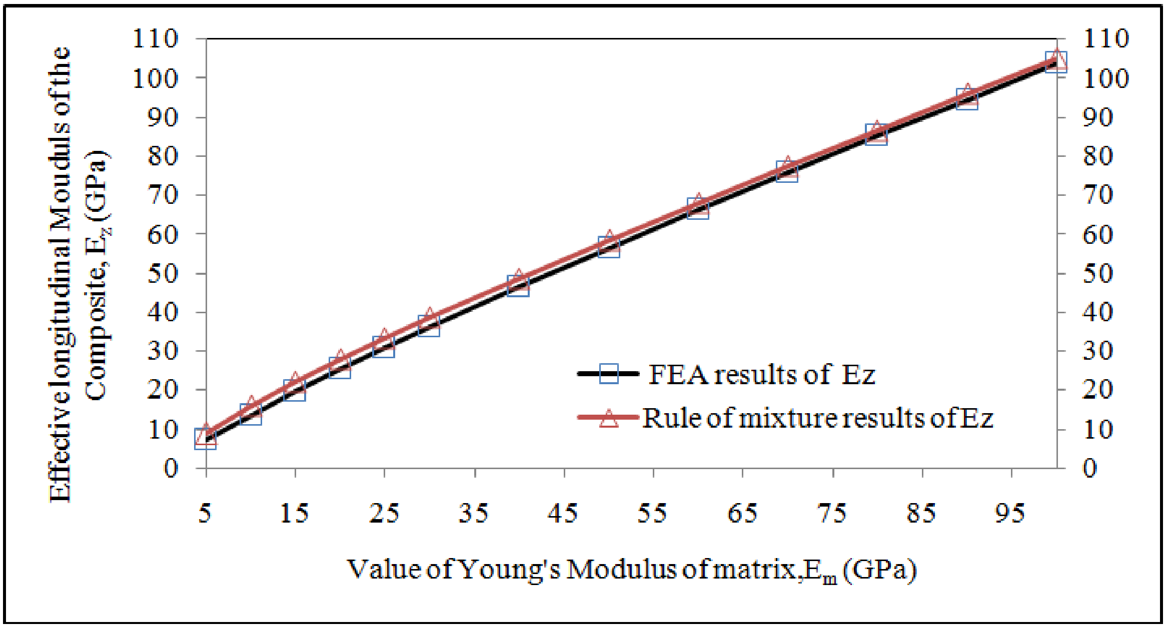

Figure 13: Comparison of Effective Modulus of the Composite in Longitudinal Direction Vs Varying Young's Modulus of the Matrix Reinforced with Short CNT of Thickness 0.4nm

H. Effect of Poisson's Ratio on the Effective Longitudinal Modulus of the Nanocomposite

Model parameters were same as long CNT. We found out that effective longitudinal modulus of the nanocomposite was remaining almost same with the increase of both Poisson's ratio of CNT and matrix. Results are calculate by increasing Poisson's ratio from .2 to 0.4 increase effective longitudinal modulus of the of nanocomposite value by 0.4422%, so we found that the effect of the Poisson ratio of the CNT and matrix on composite on the simulation was negligible which is shown in Figure 14.

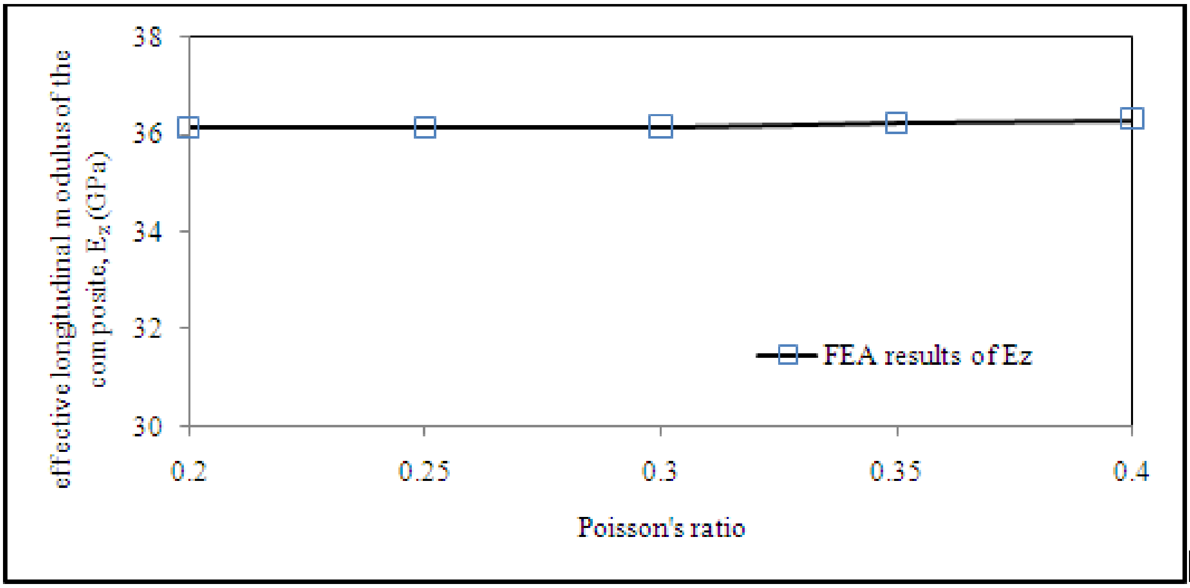

Figure 14: Effective Modulus of the Composite in Longitudinal Direction Vs Varying CNT and Matrix Poisson's Ratio with Short CNT of Thickness 0.4nm.

I. Effect of CNT Thickness on the Effective Longitudinal Modulus of the Nanocomposite

Here the modeling parameters are same as long CNT RVE. We found from Figure 15 that effective longitudinal modulus of the composite increase with the increase of thickness of CNT in short CNT case but results in FEA were not smooth as rule of mixture because in short CNT side caps produce stress concentration at two corners of short CNT. Rule of mixtures results were higher than FEA results because rule of mixture results ignore side caps of short CNT.

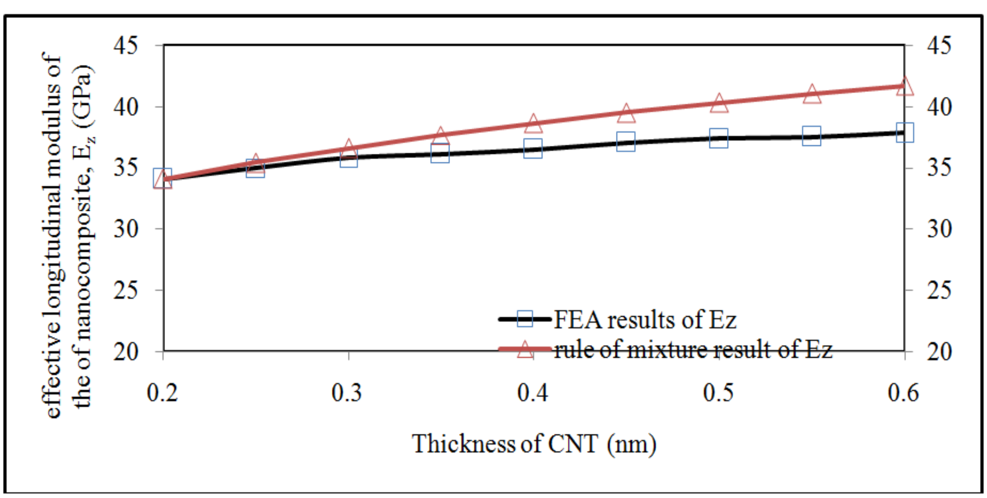

Figure 15: Effective Modulus of the Composite in Longitudinal Direction Vs Varying CNT Thickness with Short CNT.

Like long CNT, volume fraction of short CNT increases with the increases of the thickness of CNT without changing the length. Effective longitudinal modulus of the nanocomposite strongly depends on the volume fraction of CNT material. From the Figure 16 we observed that with the addition of only about 1.62% volume fraction of the CNTs in a matrix, the stiffness of the composite in the CNT axial direction can increase as much as 21.72% for the case of long CNT fibers. Variation of results between FEA and rule of mixture is large enough because rule of mixture calculation did not count the hemispherical caps of short CNT.

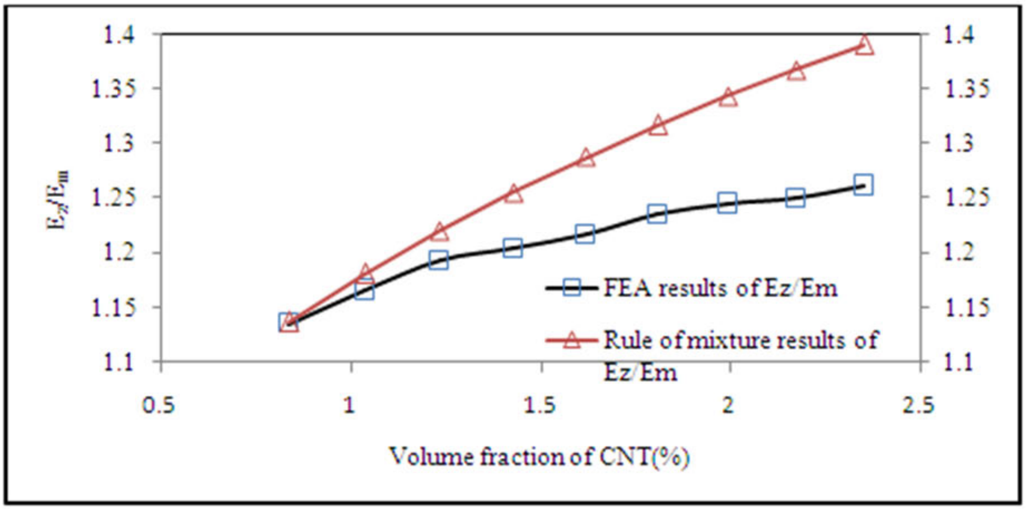

Figure 16: Comparison of Effective Modulus of the Composite in Longitudinal Direction Vs Various CNT Volume Fractions with Short CNT.

J. Effect of Interphase on the Effective Longitudinal Modulus of the Nanocomposite

In this case a layer of interphase is considered between CNT and matrix with thickness 0.40nm and Young's modulus of interphase is varied from 1 to 15 GPa. Here to find the value effective longitudinal modulus of composites, model parameters are kept same as long CNT except the length of short CNT and interphase. From Figure 17, we observe that value of E_z increase with the increase of E_i but the increase was not smoothed straight-line. Square RVE with short CNT and interphase between matrix and short CNT is still under investigation.

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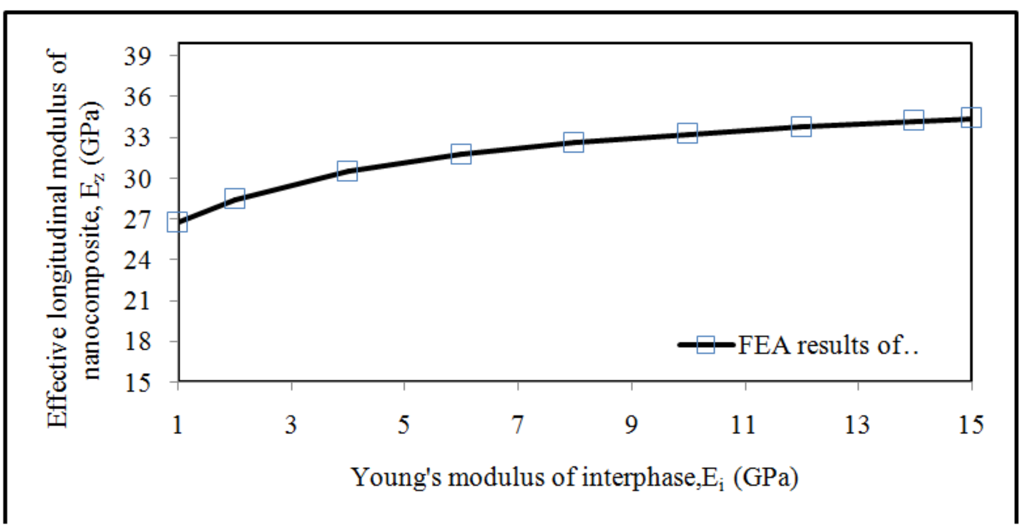

Figure 17: Effective Modulus of the Composite in Longitudinal Direction (Only FEA) Vs Varying Interphase Young's Modulus for Short CNT.

V. Conclusion

In this study, the effective Young‘s modulus of CNT-based nanocomposites has been evaluated, and as a preliminary step in this process, validation of continuum mechanics is done using 3-D square RVE models of the composite. Numerical examples using both long and short CNT-based composites have been studied and validated using the strength of materials approach. The results are in complete agreement revealing the fact that continuum mechanics can be an excellent approximate in estimating the overall response of the composite system. The FEM results evaluated assuming perfect bonding condition justifies the fact that,

1. With the increase of Young‘s modulus of matrix, the value of E_z/E_m decreases i.e. for higher Young‘s modulus of matrix, the increase in stiffness of composite is low, which is relatively higher for lower Young‘s modulus of matrix
2. Poisson‘s ratio of both CNT and matrix has almost negligible effect on the effective modulus of CNT based nanocomposite in longitudinal direction i.e. 100% increase in Poisson‘s ratio causes only 0.4704% and 0.4422% increase in the effective modulus of CNT based nanocomposite in longitudinal direction
3. With additions of only 0.40 nm of CNT thickness, effective modulus of CNT based composite in longitudinal direction increases 43.92% and 11.10% for long and short CNT respectively

And the FEM results evaluated assuming imperfect bonding condition justifies the fact that, Increase in Young‘s modulus of interphase causes increase in effective modulus of the CNT based nanocomposite in longitudinal direction for both long and short CNT but forthe short CNT the increasing rate was higher at lower valueof Young‘s modulus of interphase but that rate reduced atwith the increase of interphase Young‘s modulus.

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