

Prediction of Young's Modulus of Carbon Nanotube Reinforced Composites in Axial Direction with Nonlinear Springs

¹M.R. Davoudabadi, ²R. Ebrahimi Naghami and ¹A. Fereidoon

¹Mechanical Engineering Department, Semnan University, Semnan, Iran

²Mechanical Engineering Department, Sharekord University, Sharekord, Iran

Abstract: In this article, a molecular structural mechanics/finite element (MSM/FE) Multiscale modeling of carbon nanotube/polymer composites with linear elastic polymer matrix is introduced. The macroscopic elastic properties of carbon nanotube reinforced composites are evaluated through analyzing the elastic deformation of a representative volume element (RVE) under axial loading conditions. This RVE contains three components, carbon nanotube, interface between the nanotube and polymer matrix, we assumed to be bonded by Vander Waals interactions based on the Lennar-Jonze potential at the interface and polymer matrix. Using the MSM/FE Multiscale model, we investigated the effect of carbon nanotube on the improvement of mechanical stability of the nanocomposite. First, based on the force field theory of molecular mechanics and computational structural mechanics, an equivalent beam model is constructed to model the carbon nanotube effectively. Moreover, an efficient three dimensional eight-node brick Finite element is employed to model the polymer matrix. The macroscopic behaviors of the RVE can be evaluated through the traditional finite element method. In the numerical simulations, the influences of various important factors, such as the aspect ratio of carbon nanotube, volume fraction and geometry of RVE and material properties of polymer matrix have been investigated in detail. The results show that using carbon nanotubes, the mechanical stability of polymer materials can be improved significantly.

Key words: Polymer matrix • Carbon nanotubes • Nonlinear spring • Young's modulus • Vander Waals force • Multiscale modeling • Finite element method

INTRODUCTION

The exceptional mechanical, thermal, electrical properties, low density and high aspect ratio, exhibited by carbon nanotubes [1, 2], make them an ideal candidate for composite reinforcement, polymers are vastly used in advanced engineering applications such as parts, electronic packaging, various optical components, semiconducting material, insulating, liquid crystal display and vibration damping. Polymers are especially useful because they are easy to change into complex shapes, they are lightweight and they are relatively inexpensive. But, their applications are limited due to their low melting temperature, low stiffness, low strength and time dependent liquid-like flow. The incorporation of polymers into modern applications is ever increasing, but their mechanical behavior must be understood and quantitatively predicted before using them in both

engineer and none engineering applications. The discovery of carbon nanotubes (CNTs) by Iijima in 1991 has opened the door to enhance the mechanical properties of polymer composites by adding them to the matrix materials [3]. It has been theoretically and experimentally conformed. Although there is a lot of research [4] dealing with the elastic properties of the carbon nanotube through various means, the investigations of the mechanical properties of carbon nanotube reinforced composites have been rarely reported [5, 6]. To understand the elastic properties of nanotube reinforced composites, a fundamental challenge exists in the characterization and modeling of these materials at the Nanoscale. From the traditional theoretical frame for evaluating the macroscopic elastic properties of composites, a possible approach is to build up a representative volume element (RVE) constituted by a cylindrical body of matrix with an embedded nanotube.

However, it is almost impossible to model this RVE using the molecular dynamics directly if the matrix materials (e.g. polymer) and the nanotube are all considered. A continuum mechanics approach [5, 6] can be employed to tackle this problem, although the reflection of some important characteristics of components in composites at the level of atoms should be required. CNT based nanocomposites form a new class of lightweight super strong functional materials for structural applications, energy storage, molecular sensors and biomedical applications. Recent experimental results have demonstrated that substantial improvements in the elastic properties of a polymer can be obtained by using small volume fractions of carbon nanotubes as a reinforcing phase. Theoretical and experimental works have been done to investigate the effect of the nanotubes on the behavior of polymers. Because nanotubes are on the same length scale as polymer chains, it is assumed that the polymer segments in the vicinity of the nanotubes are identified by a mobility that is different from polymer chains in the bulk material. This reduced mobility in the local region called the interphase, results in significant differences between the behavior of the bulk polymer and that of the nanotube reinforced polymer. Computational approach can play a significant role in the development of the CNT-based composites by providing simulation results to help on the understanding, analysis and design of such nanocomposites and it can be divided into two methods; atomic methods and continuum mechanics based methods. Molecular dynamics (MD) is an accurate atomistic method in simulating the mechanical behavior of CNT-based nanocomposites. This method is limited to very small length and time scales. On the other hand, although continuum based methods have been successfully used to model the effective mechanical behavior of carbon nanostructures, their application is limited to simple nanostructure. Among the various modeling techniques, it seems that the Multiscale modeling is the most efficient method that can model the mechanical behavior of CNT based polymer nanocomposite accurately. Multiscale modeling is a combination of several modeling methods that are used to span multiple time and length scales. There are two basic Multiscale approaches; (a) hierarchical methods and (b) hybrid or concurrent methods. In hierarchical modeling, first simulations at the higher resolution are performed. Properties extracted are used as input in the next level method. In hybrid modeling, there are different methods used to describe the given regions of the material with the appropriate time and length scale resolution.

The difficulty encountered in this class of problems is that while atomistic regime is conceived as discrete set of atoms (modeled by molecular dynamics/mechanics), continuum methodologies assume the presence of a differentiable displacement field with no specific assumptions on the underlying physical matter that causes the motion [7]. Many Multiscale methods such as quasi continuum method, coarse-grained molecular dynamics and handshaking methods use intense atomic calculations near the core of atomic-scale in homogeneity and use continuum based solutions in the homogeneously deforming regions. Several groups have used the Multiscale approach for modeling the properties of CNT/polymer composite materials. Namilaie and Chandra were the first who used MD/FE Multiscale modeling to investigate these nanostructures [8]. In their work, interfaces in nanotube-based composites were modeled as hydrocarbon chemical attachments between the matrix and CNT. They used MD simulations for fiber pullout tests to understand the load transfer behavior of the CNT and quantitatively determined the interface strength. These results were used to generate a traction-displacement constitutive relation for a continuum description of interfaces in terms of cohesive zone model. Thus, a Multiscale methodology was formulated using the atomically informed cohesive zone model to represent interfaces in a finite element formulation. This Multiscale method was a hierarchical time-consuming method because of using MD to simulate the CNTs. At the Nanoscale, analytical models are difficult to establish or too complicated to solve and tests are extremely difficult and expensive to conduct. Modeling and simulations of nanocomposites, on the other hand, can be achieved readily and cost effectively on even a desktop computer. Characterizing the mechanical properties of CNT-based composites is just one of the many important and urgent tasks that simulations can accomplish. To overcome these problems, Li and Chou developed a concurrent molecular structural mechanics/finite element (MSM/FE) Multiscale method. To model the matrix, they considered the linear elastic behavior for polymer [9]. For modeling carbon nanotubes in the atomistic scale, they developed a new molecular structural mechanics (MSM) method. In this method, a single-walled carbon nanotube is viewed as a space frame, where the covalent bonds are represented as connecting beams and the carbon atoms as joint nodes. Based on the energy equivalence between local potential energies in computational chemistry and elemental strain energies in structural mechanics, the elastic constants of the equivalent beam including tensile resistance, flexural rigidity and torsional stiffness can be determined [9].

In this article, we determine the elastic behavior of carbon nanotube/polymer composites using a MSM/FE Multiscale modeling approach. The nanotube is modeled at the atomistic scale by the MSM method. The matrix deformation is analyzed at the macroscopic scale by the continuum finite element method [10, 11]. To model the mechanical properties of polymers accurately, we use the nonlinear finite element method considering behavior of interface between the nanotube and the polymer matrix. The Nanotube and polymer matrix are assumed to be bonded by Vander Waals interactions at the interface and nonlinear spring is used for simulating the Vander Waals interactions. This model is used to study the effect of CNT on the improvement of mechanical properties of the polymer matrix.

Modeling: Here, we use structural molecular mechanics to model the carbon nanotubes [12]. The element used for the covalent bonds is a uniaxial element with tension, compression, torsion and bending capabilities and has six degrees of freedom at each node; three translations in x, y, z directions and three rotations about x, y, z axes. This element is defined by the cross sectional area, the moment of inertia and the material properties. Based on the energy equivalence between local potential energies in the computational chemistry and elemental strain energies in the structural mechanics, the elastic constants for the equivalent beam are determined. The force field constants of the covalent bonds are used as follows:

$$\frac{EA}{L} = K_r, \frac{EI}{L} = k_\theta, \frac{GJ}{L} = k_\phi \quad (2.1)$$

The force field constants K_r, k_θ, k_ϕ represent stretching, bending and torsional stiffness of the covalent bonds, respectively [13]. Also, E and G denote module of elasticity and shear of the element, respectively. Moreover, A is the cross sectional area, I the moment of inertia, J the polar moment at Equation (3) and L the length of the beam.

The length of the element is assumed to be equal to the covalent distance of the carbon atoms.

$$L = a_{c-c} = 0.1421 \text{ nm}.$$

Specific parameters of the element with a circular cross section could be obtained from the Equation (1) as follow [12]:

$$d = 4\sqrt{\frac{K_\theta}{K_r}}, E = \frac{K_r^2 L}{4\pi K_\theta}, G = \frac{K_r^2 K_\tau L}{8\pi K_\theta^2} \quad (2.2)$$

$$A = \frac{\pi d^2}{4}, I = \frac{\pi d^4}{64}, J = \frac{\pi d^4}{64} \quad (2.3)$$

Where d is the cross-sectional diameter of the element. In the references of molecular mechanics, the units of the force constants K_r and K_θ are kcalmol⁻¹rad⁻², respectively. For the convenience of computation, we exchange them into nN nm⁻¹ and nN nm rad⁻², respectively. These are well-known force field constants for modeling the carbon-carbon covalent bonds in CNTs and have been demonstrated successfully for modeling the static, dynamic and thermal properties of carbon nanotubes and their composites. These values are listed as follow [12]:

$$\begin{aligned} K_r &= 6.52 \times 10^{-7} \text{ Nnm}^{-1} \\ K_\theta &= 8.76 \times 10^{-10} \text{ Nnmrad}^{-2} \\ K_\tau &= 2.78 \times 10^{-10} \text{ Nnmrad}^{-2} \end{aligned} \quad (2.4)$$

as mentioned earlier, CNTs carbon atoms are bonded together with covalent bonds forming a hexagonal lattice. These bonds have a characteristic bond length C-C and bond angle in the 3D space. The displacement of individual atoms under an external force is constrained by the bonds. Therefore, the total deformation of the nanotube is the result of the interactions between the bonds. By considering the bonds as connecting load-carrying elements and the atoms as joints of the connecting elements, CNTs may be simulated as space-frame structures. By treating CNTs as space-frame structures, their mechanical behavior can be analyzed using classical structural mechanics methods. In this work, a 3D FE model able to assess the mechanical properties of SWCNTs is proposed [12]. The 3D FE model is developed using the ANSYS commercial FE code. For the modeling of the bonds, the 3D elastic BEAM4 ANSYS element is used. The specific element is a uniaxial element with tension, compression, torsion and bending capabilities. It has six degrees of freedom at each node: translations in the nodal x, y and z directions and rotations about the nodal x, y and z-axes. The element is defined by two or three nodes as well as its cross-sectional area, two moments of inertia, two dimensions and the material properties. Prediction of material properties of nanotube, The Young's modulus of a material is the ratio of normal stress to normal strain as obtained from a uniaxial tension test. Following this definition, the Young's modulus of SWCNTs is been calculated using the following equation.

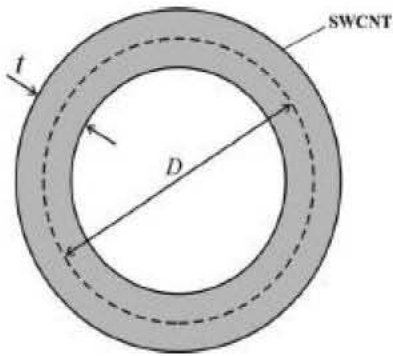


Fig. 1: Schematic of SWCNT Cross-section area

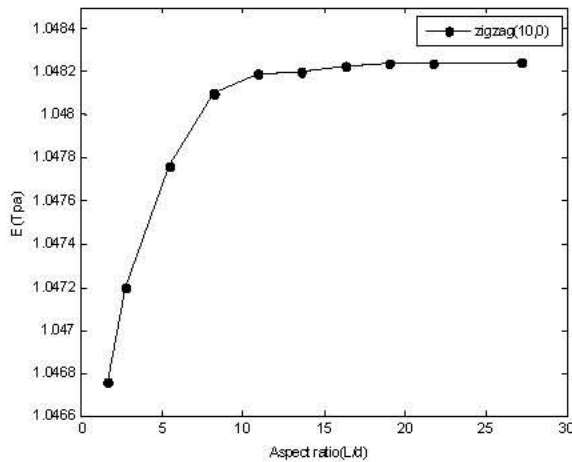


Fig. 2: Variations of Young's modulus of zigzag respect to aspect ratio

$$E_{cnt} = \frac{FL}{A_{cnt}\Delta L} \quad (2.5)$$

F is the total applied force, A_{cnt} , the cross-sectional area, L the initial length and ΔL the elongation. A_{cnt} is equal to $\pi \cdot D \cdot t$ where D is the mean diameter of the tube. It is shown in Fig. 1.

The nodes of the bottom end of the SWCNT have been fully constrain (zero displacement and rotation conditions), while the nodes of the upper end, are subjected to tensile forces. From the results it is clear that the wall thickness of CNTs significantly affect the calculation of Young's modulus of SWCNTs. The larger the wall thickness, the smaller the Young's modulus calculated. In the current work, energy equivalence between molecular and structural mechanics provides a wall thickness of 0.34nm. the results of present model are shown for zigzag (10, 0) and armchair (10, 10) in Figs 2 and 3. The present Young's modulus of nanotube is in good agreement with the many previous theoretical

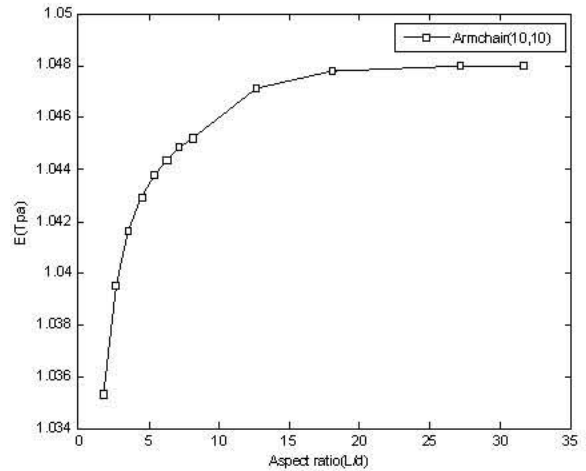


Fig. 3: Variations of Young's modulus of armchair respect to aspect ratio

predictions and experimental results [14-21]. Note that the currently existing theoretical and experimental values of the Young's modulus is quite scattered. The Young's modulus of nanotube ranges from 1 to 1.05 TPa, from the different references. The Young's modulus of zigzag nanotube is greater than armchair nanotube modulus.

The MSM model for prediction of the carbon nanotube can be adopted into a finite element model for prediction of the mechanical properties of nanotube reinforced composites. Continuum-based FE formulation is implemented to analyze the interphase layer and outer polymer matrix. Here, an isoparametric cubic element is used for modeling the matrix. The element is defined by eight nodes having three degrees of freedom per node: three x, y and z directions. The polymer matrixes selected in this study are poly ethylene amorphous, crystalline poly ethylene. The Young's modulus of this isotropic amorphous polymer is assumed to be 3 GPa and Poisson's ratio is chosen as 0.3. The nanotube and matrix are assumed to be bonded by Vander Waals interactions based on the Lennars-Jones (LJ) potential at the interface [22]. For modeling these forces, nonlinear spring elements are implemented in this work. The spring element used here is defined by two nodes and a spring constant. To construct these elements, the distances between the nodes on CNT wall and the nodes on the inner surface of the polymer matrix are computed because of the matrix is continuum and each nodes on CNT connected to three node at inner wall of matrix we assumed that stiffness of equal spring is 3K. A spring element is inserted between every two nodes with their distance smaller than the cut off radius of LJ potential. It is a uniaxial tension – compression element with three degrees of freedom at each

node: three translations in the x, y and z directions. No bending or torsion is considered in this element. The spring stiffness of this element is determined by the second derivative of the LJ potential [23], as follows:

$$V_{LJ} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (2.6)$$

$$K = \frac{d^2 V_{LJ}(r)}{dr^2} = \frac{624\epsilon\sigma^{12}}{r^{14}} - \frac{168\epsilon\sigma^6}{r^8} \quad (2.7)$$

Where r is inter atomic distance and ϵ and σ are the LJ parameter. For carbon-carbon Vander Waals interactions, these parameters are as follows:

$$r = \sqrt[6]{2}\sigma \quad (2.8)$$

$$\epsilon_{c-ch_2} = 0.004556, \sigma_{c-ch_2} = 0.3825 \quad (2.9)$$

For obtaining the Young's modulus of polymer nanocomposite we considered two models one of them the long CNT through the polymer matrix and another is a short CNT with cap inside the polymer matrix. The thickness of the interphase layer is assumed to be 0.4293nm, based on previous molecular mechanics works. The cross section of the unit cell is dependent on the CNT volume fraction in the RVE. The CNT volume fraction (V_f) is an important variable in determining the composite mechanical properties and can be defined [24]:

$$V_f = \frac{\pi \left(R_{cnt} + \frac{h_{vdw}}{2} \right)^2}{A_{cell}} \quad (2.10)$$

Where h_{vdw} is the equilibrium Vander Waals separation distance between the CNT and the matrix and A_{cell} is the cross-sectional area of the unit cell. It can be expressed as:

$$A_{cell} = \pi(R_m^2 - R_{cnt}^2) \quad (2.11)$$

The Vander Waals separation distance depends on the nature of the CNT-polymer interfacial interactions and is assumed to 0.4293nm. We applied the armchair and zigzag nanotubes through the polymer matrix.

To study the effect of volume fractions and diameter and length of nanotube on the Young's modulus of the polymer nanocomposite, after constructing the RVE, we impose load in the RVE and the macroscopic behavior of the RVE can be evaluated using the FE method.

RESULTS AND DISCUSSION

Using the MSM approach and nonlinear finite element method, computational modeling of a continuous CNT/polymer composite has been carried out in this work. This Multiscale modeling approach is implemented to study the mechanical properties of the polymer matrix nanocomposite under axial tensile loading. When considering the tube as a solid shell body, from the classical elastic, we assumed the deformation of nanocomposite is Isostrain; the results are compared with Rule of mixture. The rule of mixture can be expressed as:

$$E_z = E_f V_f + E_m (1 - V_f) \quad (3.1)$$

Where E_f and E_m are in order to nanotube modulus and matrix modulus and V_f is volume fraction. Isostrain assumption led to:

$$\frac{F_m}{A_m E_m} = \frac{F_{cnt}}{A_{cnt} E_{cnt}} \quad (3.2)$$

F_m is the load that exert on cross- section area of matrix and F_{cnt} is the load of nanotube. E_m is the Young's modulus of polymer matrix. By applying the elastic relation of displacement Fig. 3, we will have:

$$E_c = \frac{F_{total} L}{A_{eq} \Delta L} \quad (3.3)$$

Where E_c is the Young's modulus of nanocomposite in the longitudinal direction, ΔL is elongation in z direction; F_{total} is the total load that exerted on nanocomposite that expresses by following Equation:

$$F_{total} = F_{cnt} + F_m \quad (3.4)$$

The A_{eq} is the nanocomposite cross section area.it can be expressed as:

$$A_{eq} = \pi(R_m^2 - R_{cnt}^2) + \pi D_{cnt} t \quad (3.5)$$

The Poisson's ratio in zx plane is obtained

$$\nu_{zx} = -\frac{\Delta R}{R} \bigg/ \frac{\Delta L}{L} \quad (3.6)$$

For short nanotube inside the polymer matrix, after applying tension force Fig. 5, the displacement in z direction determined by traditional Finite element method, Δ is the displacement and we will obtain the Young's modulus of composite part as follow:

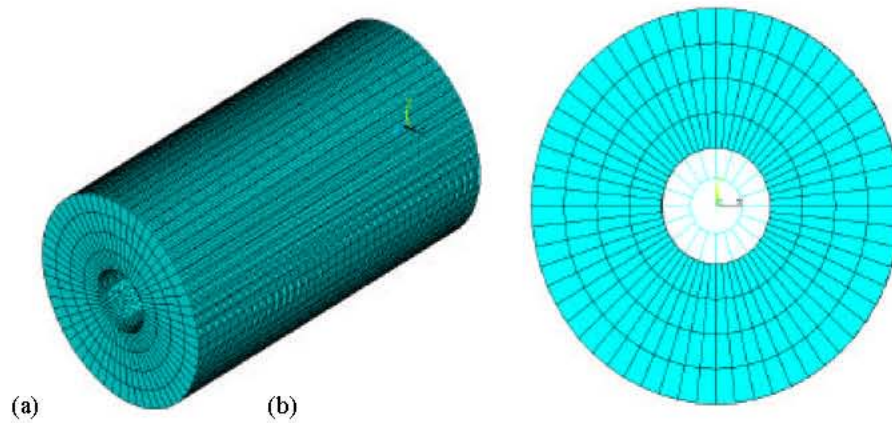


Fig. 4: Finite element macroscopic model for CNT/polymer composite. CNT through the RVE a) Isometric view b) left view

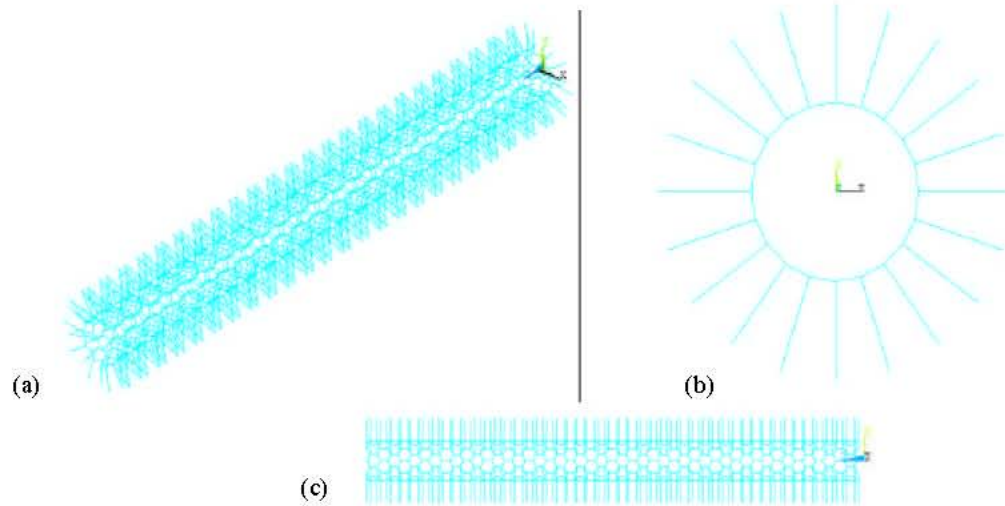


Fig. 5: The schematics of spring elements on nodes of CNT wall a) isometric view b) Left view. c) Front view

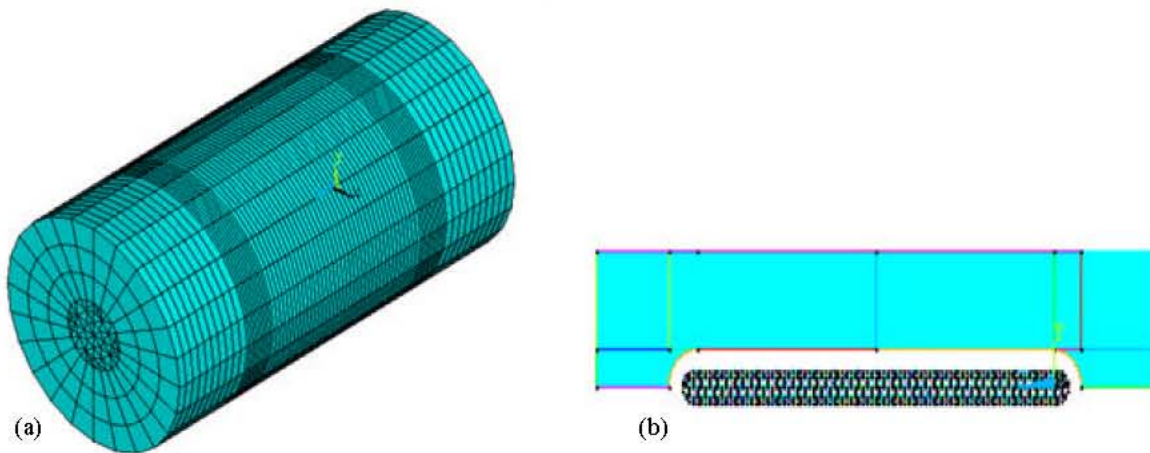


Fig. 6: Computational model for CNT/polymer composite. CNT inside the RVE a) isometric view b) a cylindrical RVE shown in a cut-through view.

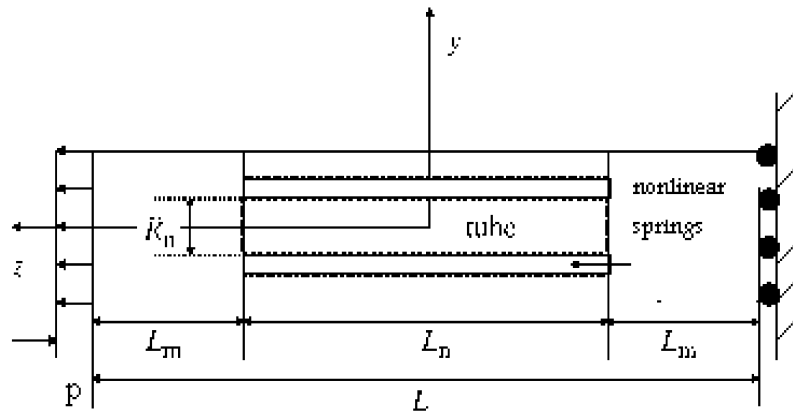


Fig. 7: For the case of the nanotube embedded inside the RVE

$$\delta = \frac{P2L_m}{AE_m} + \frac{PL_n}{A_nE_c} \quad (3.7)$$

Where L_m is the polymer matrix and p is tension force L_n is the composite part length, A_n and A are defined as:

$$A_n = \pi(R_m^2 - R_{cnt}^2), \quad A = \pi R_m^2 \quad (3.8)$$

For the case of the nanotube embedded inside the RVE in Fig 4, with the assumption of perfect bonding between the nanotube and matrix, [6] gave out the expression of the effective Young's modulus as follows:

$$\frac{1}{E_z} = \frac{2}{E_m} \left(\frac{L_m}{L} \right) + \frac{1}{E_c} \left(\frac{A}{A_n} \right) \left(\frac{L_n}{L} \right) \quad (3.9)$$

After determining the properties of nanotube and nonlinear spring interaction between the nanotube and polymer matrix, the material properties of the nanotube reinforced composites can be predicted. Our numerical simulation is concentrated on the two case of polymer matrix reinforced with unidirectional short nanotubes inside the matrix and long nanotube through polymer matrix. This may be the ultimate goal for reinforcement. In this case, the RVE of our FEM model is shown in Fig2. For the polymer matrix, its Poisson ratio ν_m is chosen as 0.3. [25] The Young's modulus of polymer E_m is quite scattered, depending on the various structures. Here, we take it as 0.5 GPa in our Computation. When the volume fraction varies from 0.211 to 0.48%, the increase in E_z is occurred. this variation for different zigzag nanotubes are shown respect to aspect ratio in Fig5 It is shown by increasing in chirality of zigzag the value of Young's module is decreased. The reason is increasing in diameter of nanotube (the increase of the stiffness in the CNT

cannot compensate the loss of material due to the increased diameter). the volume fraction of nanotube in matrix increased from 0.0211 to 0.048 and the stiffness of nanocomposite in axial direction can increase, this result is shown in Fig 6.

The effect of different volume fraction respect to the aspect ratio is shown in Fig 7. The effects of different Young modules of polymer matrix are shown in Figs 8 and 9 respects to aspect ratio. If we apply the armchair nanotube for reinforcement of polymer matrix the value of Young's modulus is decreased, because the Young's modulus of zigzag is greater than Armchair. It is shown in Figs 10 and 11.

The results of this study show that the effective Young's modulus obtained from current model is less than that predicted by Rule of Mixtures. Our model also predicts that by increasing the volume fraction of CNT in composite, the difference between Young's modulus of current model and that of the Rule of Mixtures' modulus will increase. The reason of overestimation of Young's modulus by Rule of Mixtures comparing to current model is the assumption of perfect bonding in Rule of Mixtures. Moreover, it is shown here that by increasing the RVE length and thus the CNT aspect ratio, closely predicts the Young's modulus introduced by Rule of Mixtures.

Next, an RVE for a short CNT in a matrix as shown in Fig 4 is studied. All dimensions for RVE are the same as in the previous, with the two hemispherical end caps. The material constants used for the CNT and matrix are the same as in the first example. Coupled DOF constraint is imposed for the surface under the axial load. The effects of volume fraction are shown in Figs 13 and 14. It is expressed the value of Young's modulus is increased by increasing the volume fraction. The amount of strength is not the same as the pervious examples

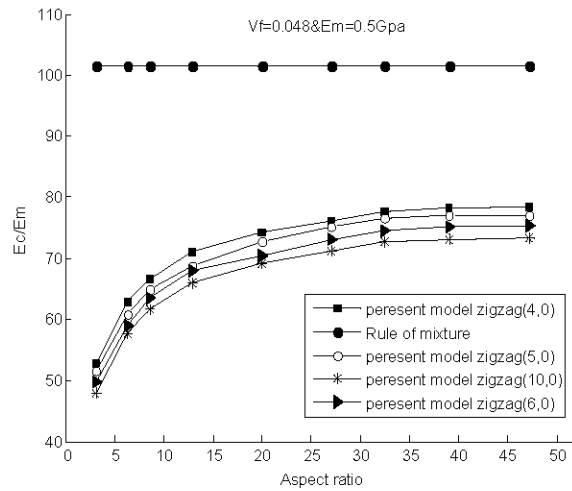


Fig. 8: Variations Young's modulus RVE for different zigzag nanotube respect to aspect ratio and compare with rule of mixture, ($V_f=0.048$ and $E_m=0.5\text{GPa}$)

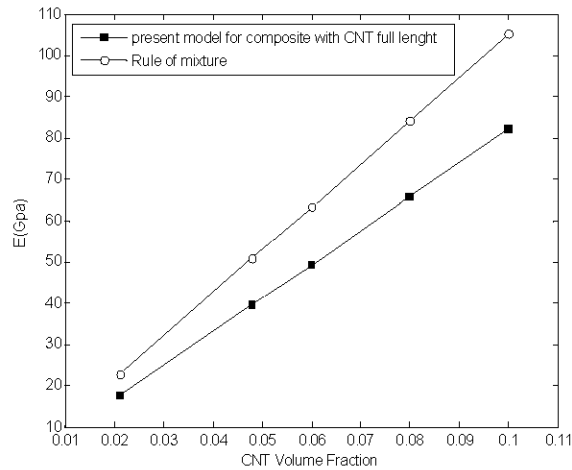


Fig. 9: Young's modulus of nanocomposite for different volume fractions and compared with rule of mixture.

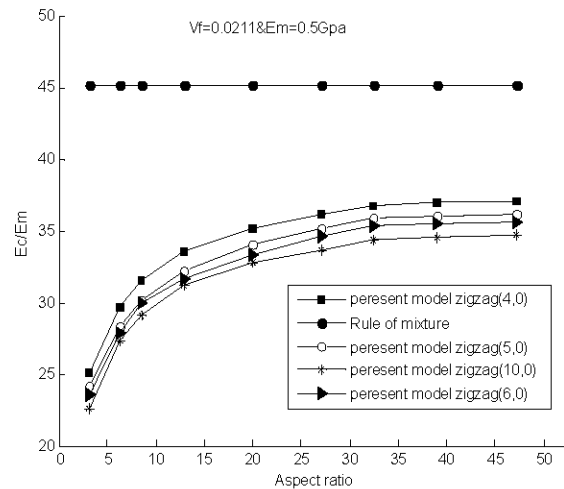


Fig. 10: Variations Young's modulus RVE for different zigzag nanotube respect to aspect ratio and compare with rule of mixture, ($V_f=0.0211$ and $E_m=0.5\text{GPa}$).

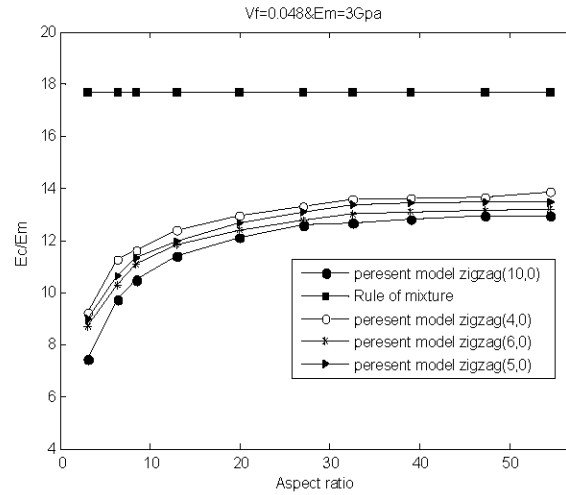


Fig. 11: Variations Young's modulus RVE for different zigzag nanotube respect to aspect ratio and compare with rule of mixture, ($V_f=0.048$ and $E_m=3.0$ GPa)

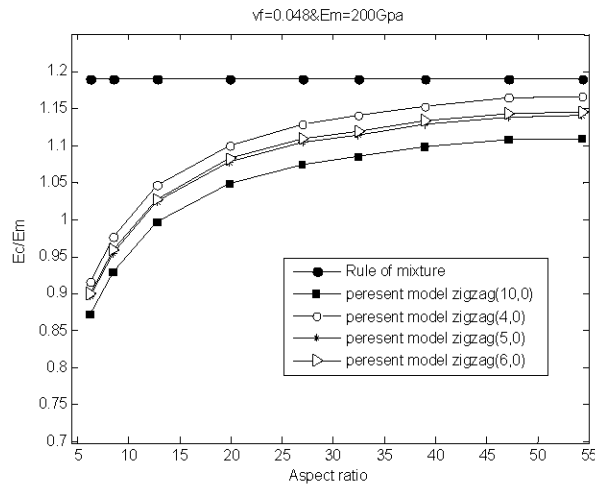


Fig. 12: Variations Young's modulus RVE for different zigzag nanotube respect to aspect ratio and compare with rule of mixture, ($V_f=0.048$ and $E_m=200$ GPa)

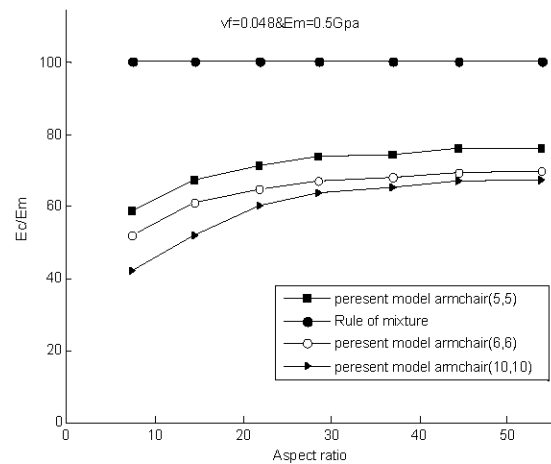


Fig. 13: Variations Young's modulus RVE for different armchair nanotube respect to aspect ratio and compare with rule of mixture, ($V_f=0.048$ and $E_m=0.5$ GPa)

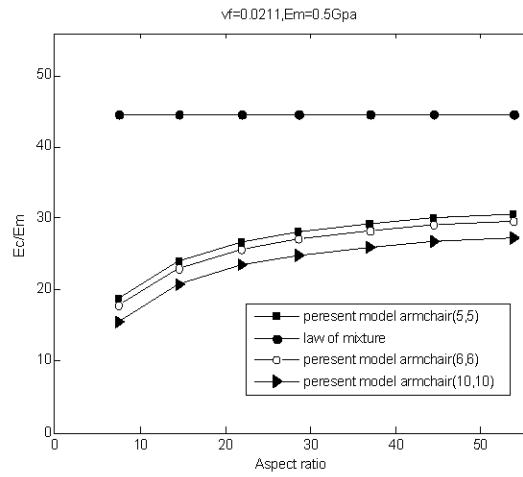


Fig. 14: Variations Young's modulus RVE for different armchair nanotube respect to aspect ratio and compare with rule of mixture, ($V_f=0.0211$ and $E_m=0.5\text{GPa}$)

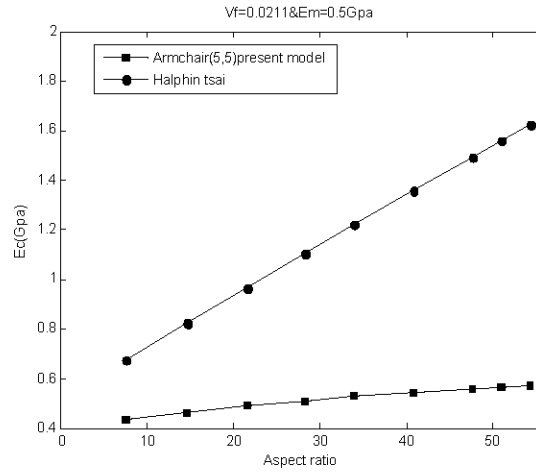


Fig. 15: Variations Young's modulus RVE for different armchair nanotube respect to aspect ratio and compare with Halphin Tsai, ($V_f=0.0211$ and $E_m=0.5\text{GPa}$)

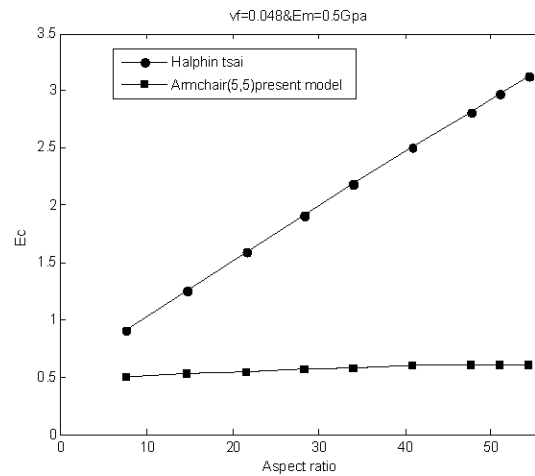


Fig. 16: Variations Young's modulus RVE for different armchair nanotube respect to aspect ratio and compare with Halphin Tsai, ($V_f=0.0211$ and $E_m=0.5\text{GPa}$)

because the increase of the stiffness in the CNT cannot compensate the loss of the material due to the reduced volume. These simulations are very good agreement with experimental works [26]. All these results suggest that short CNTs in a matrix may not be as effective as long CNTs in reinforcing the composites. The Halpin Tsai relations are as follow:

$$E_L = \left(\frac{1 + 2\left(\frac{L_f}{d_f}\right)\eta_L v_f}{1 - \eta_L v_f} \right) E_m \quad (3.10)$$

L_f is the length of CNTs in the matrix; d_f is the diameter of CNTs. η_L is defined as follow:

$$\eta_L = \frac{\left(\frac{E_f}{E_m}\right) - 1}{\left(\frac{E_f}{E_m}\right) + 2\left(\frac{L_f}{d_f}\right)} \quad (3.11)$$

By increasing the aspect ratio, after a value the Young's modulus is fixed and the increase of length is not effective on it. For increasing CNTs diameter the value of Young's modulus is reduced. Many research issues need to be addressed in the modeling and simulations of CNTs in a matrix material for the development of nanocomposites. Analytical methods and simulation models to extract the mechanical properties of the CNT-based nanocomposites need to be further developed and verified with experimental results. The simulation approach developed in this paper is only a tool for understanding the mechanical behavior of this new material. Different interface conditions, other than perfect bonding, need to be investigated using different models to more accurately account for the Nanoscale. Single wall and multi wall CNTs are reinforcing fibers in a matrix can be studied by simulations to find out their advantages and disadvantages. These simulation results, which are believed to be the first of its kind for CNT-based composites, are consistent with the experimental results reported in the literature [27-30]. Finally, large Multiscale simulation models at the nano, micro and macro scales, need to develop. Interactions among a large number of CNTs in a matrix can be simulated if the computing power is available.

CONCLUSION

The elastic properties of carbon nanotube-reinforced composites are predicted in this paper through analyzing the elastic deformation of a RVE under axial loading cases. To construct this RVE, consisting of the carbon nanotube, the interaction between the nanotube and the polymer matrix constructed with nonlinear springs, first, an equivalent beam model for carbon nanotube is built up. For the modeling of the bonds, the 3D elastic BEAM4 ANSYS element is used. The explicit relationships between the material properties of the equivalent beam element and the force constants have been derived. Second, to describe the interaction between the nanotube and the polymer matrix at the level of atoms, the molecular mechanics and molecular dynamics computations have been performed to obtain the thickness and material properties of the CNTs. The Lenard Jonze potential force is used for simulating interaction, Vander Waals forces by nonlinear springs. Moreover, an efficient 3D eight-node brick finite element is employed to Model the matrix. Consequently, the macroscopic behaviors of the RVE can be evaluated using the traditional FEM. From the predicted results, the following conclusions can be made. When using Lenard-Jones type potentials, the stiffness of nonlinear strongly depends on the deformation in a form of nonlinearity. These bonds simulated Vander Waals force, is very weak and in the short length of CNT did not transient the force to matrix and reflect. Increase in nanotube length leads to higher reinforcement in the nanotube length direction. Hence, the volume fraction ranges from 0.211 to 0.48%, depending on the stiffness of Vander Waals forces, because the number of this bond increased. When the Young's modulus of polymer matrix ranges from 0.5 to 200 GPa, it can result in significantly Lower E_z . However, when difference between E_m and E_{cnt} is higher, the effect of nanocomposite reinforcement becomes high.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the Semnan University for supporting this research.

REFERENCES

1. Selmi, A., C. Friebel, I. Doghri and H. Hassis, 2006. Prediction of the elastic properties of single walled carbon nanotube reinforced polymers A comparative study of several micromechanical models.

2. Odegard, G.M., T.S. Gates, L.M. Nicholson and K.E. Wise, 2002. Equivalent-continuum modeling of nano-structured materials. *Compos. Sci. Tech.*, 62: 1869-1880.
3. Iijima, S., 1991. Helical microtubules of graphitic carbon. *Nature*, 354: 568.
4. Qian, D., G.J. Wagner, W.K. Liu, M.F. Yu and R.S. Rouff, 2002. Mechanics of carbon nanotubes. *Appl. Mech. Rev.*, 22: 495-533.
5. Thostenson, E.T., C. Li and T.W. Chou, 2002. Carbon nanotube-reinforced composites: processing, modeling and property characterization. In *Proceedings of the tenth US-Japan conference on composite materials*, Stanford, 16-18, September, pp: 641-647.
6. Liu, Y.J. and X.L. Chen, 2003. Evaluations of the effective material properties of carbon nanotube based composites using a Nanoscale representative volume element. *Mech. Mater.*, 35: 69-81.
7. Barber, A.H., S.R. Cohen and H.D. Wagner, 2003. Measurement of carbon nanotube-polymer interfacial strength. *Appl. Phys. Lett.*, 82: 4140-4142.
8. Namilaee, S. and N. Chandra, 2005. *J. Eng. Mater. Technol.*, 127: 222.
9. Li, C. and T.W. Chou, 2003. A structural mechanics approach for the analysis of carbon nanotubes. *Int. J. Solids Struct.*, 40: 2487-2499.
10. Liu, Y.J. and X.L. Chen, 2004. Square representative volume elements for evaluating the effective material properties of carbon nanotube-based composites.
12. Tserpes, K.I. and P. Papanikos, 2005. Finite element modeling of single-walled carbon nanotubes.
13. Sakhaee-pour, A., *et al.*, 2008. vibrational analysis of single layered grapheme sheets. *Nanotechnol.*, 19: 085702.
14. Lu, J.P., 1997. The elastic properties of single and multilayered carbon nanotubes. *J. Phys. Chem. Solids*, 58: 1649-1652.
15. Hernandez, H., C. Goze, P. Bernier and A. Rubio, 1998. Elastic properties of C and B_x C_y N_z composite nanotubes. *Phys. Rev. Lett.*, 80: 4502-4505.
16. Chopra, N.G. and A. Zettl, 1998. Measurement of the elastic modulus of a multi-wall boron nitride nanotube. *Solid State Commun.*, 105: 297-300.
17. Krishnan, A., E. Dujardin, T.W. Ebbesen, P.N. Yianilos and M.M.J. Treacy, 1998. Young's modulus of single-walled nanotubes. *Phys. Rev. B*, 58: 14 013-14 019.
18. Salvetat, J.P., J.M. Bonard, N.H. Thomson, A.J. Kulik, L. Forro, W. Benoit and L. Zuppiroli, 1999. Mechanical properties of carbon nanotubes. *Appl. Phys. A.*, 69: 255-260.
19. Jin, Y. and F.G. Yuan, 2002. Elastic properties of single-walled carbon nanotubes. In *43rd AIA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference*.
20. Popov, V.N., V.E. Van Doran and M. Balkanski, 2000. Elastic properties of single-walled carbon nanotubes. *Phys. Rev. B*, 61: 3078-3084.
21. Chang, T.C. and H.J. Gao, 2003. Size-dependent elastic properties of a single-walled carbon nanotube via a molecular mechanics model. *J. Mech. Phys. Solids*, 51: 1059-1074.
22. Frankland, S.J.V., A. Caglar, D.W. Brenner and M. Griebel, 2002. Molecular simulation of the influence of chemical cross-links on the shear strength of carbon nanotube-polymer interfaces. *J. Phys. Chem. B*, 106: 3046-3048.
23. Montazeri, A. and R. Naghdabadi, 2009. study the effect of Viscoelastic matrix model on the stability of CNT/polymer composites by Multiscale modeling, polymer composites.
24. Gates, T.S., G.M. Odegard, S.J.V. Frankland and T.C. Clancy, 2005. Computational Materials: Multi-scale modeling and simulation of nanostructure materials, *Comp. Sci. Tech.*, 65(2): 2416-2434.
25. Han, Y. and J. Elliott, 2005. Molecular dynamics simulations of the elastic properties of polymer/carbon nanotube composites. *Comput. Mater. Sci.*, 9: 34-44.
26. Schadler, L.S., S.C. Giannaris and P.M. Ajayan, 1998. Load transfer in carbon nanotube epoxy composites. *Applied Physics Lett.*, 73(26): 3842-3844.
27. Guzmán de Villoria, R. and A. Miravete, 2007. Mechanical model to evaluate the effect of the dispersion in nanocomposites *Acta Materialia*, 55: 3025-3031.
28. Bower, C., R. Rosen, L. Jin, J. Han, *et al.*, 1999. Deformation of carbon nanotubes in nanotube-polymer composites. *Appl. Physics Lett.*, 74(22): 3317-3319.

29. Wagner, H.D., O. Lourie, Y. Feldman and R. Tenne, 1998. Stress-induced fragmentation of multiwall carbon nanotubes in a polymer matrix. *Appl. Physics Lett.*, 72(2): 188-190.
30. Qian, D., E.C. Dickey, R. Andrews and T. Rantell, 2000. Load transfer and deformation mechanisms in carbon nanotube polystyrene composites. *Appl. Physics Lett.*, 76(20): 2868-2870.