Investigation of the Interphase Effects on the Mechanical Behavior of Carbon Nanotube Polymer Composites by Multiscale Modeling

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Received 5 March 2009; accepted 12 September 2009
DOI 10.1002/app.31460
Published online 17 March 2010 in Wiley InterScience (www.interscience.wiley.com).

ABSTRACT: In this article, a multiscale modeling procedure is implemented to study the effect of interphase on the Young's modulus of CNT/polymer composites. For this purpose, a three-phase RVE is introduced which consists of three components, i.e., a carbon nanotube, an interphase layer, and an outer polymer matrix. The nanotube is modeled at the atomistic scale using molecular structural mechanics. Moreover, three-dimensional elements are employed to model the interphase layer and polymer matrix. The nanotube and polymer matrix are assumed to be bonded by van der Waals interactions based on the Lennard-Jones potential at the interface. Using this Molecular Structural Mechanics/Finite Element multiscale model, we investigate the macroscopic material properties of nanocomposite with and without considering the interphase and compare the results with molecular dynamics (MD) simulations. It is shown that there is a noticeable deviation from MD results with two-phase model. Meanwhile, the three-phase modeling shows that by considering the effect of the interphase, the elastic constants of these nanocomposites could be calculated the same as the MD results with maximum deviation of 1.8% and negligible computational cost in comparison with the MD simulation. Hence, considering the interphase layer in modeling the CNT-based nanocomposites is necessary and cannot be ignored. © 2010 Wiley Periodicals, Inc. J Appl Polym Sci 117: 361–367, 2010

Key words: CNT-based nanocomposites; interphase; multiscale modeling; carbon nanotube; Young's modulus

INTRODUCTION

The discovery of carbon nanotubes (CNTs) has opened the door to enhance the mechanical properties of polymer composites by adding them to the matrix materials. CNTs, comprising long, thin cylinders of carbon with multiple wall layers, were first recognized in 1991 by Iijima,[1] and later found as single wall entities.[2] In addition to various experimental studies, computational modeling techniques have confirmed that CNTs possess remarkable mechanical properties such as high stiffness and strength. These properties as well as their high-aspect ratio and low density make CNTs as ideal reinforcing elements in composite nanostructured materials. CNT-based polymer nanocomposites form a new class of lightweight super strong functional materials for structural applications, energy storage, molecular sensors, and biomedical applications.[3]

Recent experimental observations have demonstrated that substantial improvements in the elastic properties of a polymer can be obtained by using small volume fractions of CNTs as a reinforcing phase.[4–6] However, since it is difficult to control and measure many of these properties experimentally, computational modeling can provide some crucial insights.[7–9] The computational approaches used for modeling the mechanical behavior of nanostructures, can be divided into two methods; atomistic methods and continuum mechanics-based methods.[10,11]

Among the various modeling techniques, it seems that multiscale modeling is the most efficient method that can model the mechanical behavior of CNT-based polymer nanocomposites accurately. Multiscale modeling is a combination of several modeling methods that are used to span multiple time and length scales.[12] 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 and properties extracted are used as input in the next level method. Hybrid methods seek to incorporate aspects of various size scale phenomena in a single simulation. Such techniques are particularly useful for simulating the behavior of structures with multiple length scale

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geometries, such as thin films, nanocomposites, and material fracture.[13]

The performance of CNT-based composites is greatly affected by the interphase, a part of matrix surrounding the nanotube, which has different properties from those of matrix and nanotube. Some theoretical and experimental works have been done to investigate the effect of the interphase on the mechanical properties of these nanocomposites.[14,15] Because the nanotubes are on the same length scale as the polymer chains, it is assumed that the polymer segments in the vicinity of the nanotubes will be identified by a mobility that is different from that of the polymer chains in the bulk material.[16] This reduced mobility with nonbulk polymer behavior is referred to the interphase. There are two main approaches in developing models used to calculate nanocomposite elastic properties, namely two and three-phase models, without and with considering the nanotube/matrix interphase, respectively.[17] Xiang et al.[18] have compared the results of several theoretical two-phase models with those of an experimental study. They found that there is no good agreement between theoretical and experimental data due to neglect of the interphase. Also, other studies have shown that the predictions of three-phase models are usually more in agreement with experimental results than those of two-phase models.[19–22] To estimate the mechanical properties of the interphase, several mathematical, experimental, and finite element approaches have been carried out.[18] Saber-Samandari and Afaghi-Khatibi[23] developed a three-dimensional unit cell model for modeling three constituent phases including nanotube, interphase and matrix. They evaluated the elastic modulus of the interphase as a function of radius and showed the effect of the interphase thickness as well as nanotube and matrix elastic moduli on the interphase properties and the overall behavior of the nanocomposites. It is to be noted that in their approach, the CNT has been modeled as a continuous medium and the mechanical properties of the nanocomposite has been calculated through a modified rule of mixtures method.

The objective of the present article is to analyze the effect of CNT/matrix interphase on the effective elastic moduli of the CNT-reinforced polymer composites using a new three-phase MSM/FE multiscale model. Although previous studies have discussed the role of the interphase layer on the elastic constants of nanocomposites, but in this work, this subject is considered quantitatively. For this purpose, the nanotube is modeled at the atomistic scale by the molecular structural mechanics method. Meanwhile, the matrix deformation is analyzed at the macroscopic scale by the continuum finite element method. In this multiscale method, the nanotube and polymer matrix are assumed to be bonded by van der Waals interactions at the interface. Also, to model the elastic properties of the interphase layer between CNT and polymer matrix in the RVE, we employ a mathematical procedure. Finally, the macroscopic elastic properties of nanotube reinforced composites have been calculated using this RVE. To find the effect of the interphase on these properties, the results obtained from two-phase and three-phase modeling (without and with considering interphase layer) are compared with a full molecular dynamics (MD) analysis of these nanocomposites.

MODELING

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 cubic body of matrix with an embedded nanotube. In a similar manner, the elastic properties of CNT/polymer composites are predicted in this article through studying the elastic deformation of a RVE under tensile loading case. To study the effect of interphase on the elastic properties of these nanostructures in this work, two distinct RVEs are used with and without considering interphase as the transition layer between the CNT and polymer matrix. These two-phase and three-phase RVEs are shown schematically in Figure 1. The three-phase RVE consists of the CNT, the transition layer between nanotube and polymer matrix and the outer polymer matrix. To construct this RVE, first, molecular structural mechanics is implemented to model the CNT in atomic scale.[24,25] In this method, a single-walled CNT 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 can be determined. 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, and z directions and three rotations about x, y, and z axes. This element is defined by cross-sectional area, moment of inertia, and material properties based on the energy equivalence between local potential energies in computational chemistry and elemental strain energies in structural mechanics. To this end, the force field constants of the covalent bonds are used as follows:

$$\frac{EA}{L} = K_r, \quad \frac{EI}{L} = K_\theta, \quad \frac{GJ}{L} = K_\phi \tag{1}$$

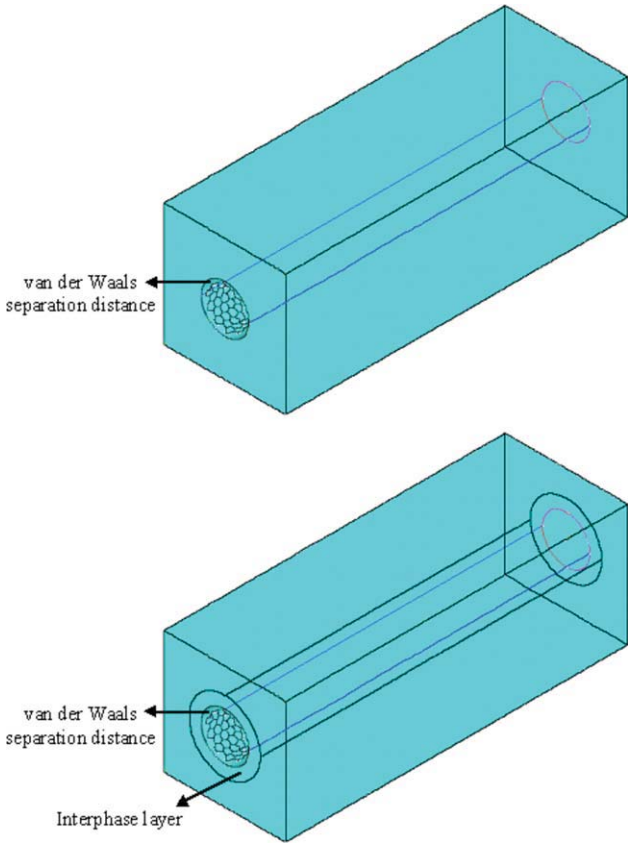

Figure 1 Schematic of two-phase and three-phase RVEs of CNT/polymer nanocomposite. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

where the force field constants K_r, K_θ, and K_ϕ, represent stretching, bending, and torsional stiffness of the covalent bonds, respectively. Also, E and G denote moduli of elasticity and shear of the element, respectively. Moreover, A is the cross-sectional area, I the moment of inertia, J the polar moment, 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 (0.142 nm). Specific parameters of the element with a circular cross-section could be obtained from eq. (1) as[26]:

$$d = 4\sqrt{\frac{K_\theta}{K_r}}, \quad E = \frac{K_r^2 L}{4\pi K_\theta}, \quad G = \frac{K_r^2 K_\phi L}{8\pi K_\theta^2} \tag{2}$$

where d is the cross-sectional diameter of the element. Usually, in the references of molecular mechanics, the units of the force constants K_r and K_θ are kcal mol^{-1} Å^{-2} and kcal mol^{-1} rad^{-2}, respectively. For the convenience of computation, we change units into nN nm^{-1} and nN nm rad^{-2}, respectively. Here, the force field constants obtained experimentally in the context of chemistry by Cornell et al.[27] in 1995 are used. These are well-known force field constants for modeling the carbon–carbon covalent bonds in CNTs and have been used successfully for modeling the static, dynamic, and thermal properties of CNTs and their composites.[24–26,28–30] These values are listed in Table I. The present molecular structural mechanics model of the CNT can be adopted into a finite element model for prediction of the mechanical properties of nanotube reinforced composites. In this manner, we can obtain these properties based on the interatomic interactions of CNT atoms with negligible computational cost.

As mentioned before, continuum-based finite element 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 translations in x-, y-, and z-directions. The nanotube and polymer matrix are assumed to be bonded by van der Waals interactions based on Lennard-Jones potential at the interface. For modeling these forces, spring elements are implemented in this work. The spring element used here is defined by two nodes and a spring constant. It is a uniaxial tension-compression element with three degrees of freedom at each node; three translations in 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, as follows:

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{3}$$

$$k = \frac{d^2 V_{LJ}(r)}{dr^2} = \frac{624\varepsilon\sigma^{12}}{r^{14}} - \frac{168\varepsilon\sigma^{6}}{r^{8}} \tag{4}$$

where r is the interatomic distance, and ε and σ are the Lennard-Jones parameters. For nonbonded carbon–carbon van der Waals interactions, these parameters are $\varepsilon = 0.0556$ kcal/mol and $\sigma = 3.4$ Å.[24] Substitution of these values in eq. (4) yields the spring stiffness of the interface elements as follows:

$$k = \frac{574.89188 \times 10^{-9}}{r^{14}} - \frac{1.00193 \times 10^{-4}}{r^{8}} \left[\frac{\text{nN}}{\text{nm}}\right] \tag{5}$$

As the main goal, we want to study the effect of interphase on the elastic modulus of the

TABLE I
Force Field Constants of the Carbon–Carbon Covalent Bonds[27]

K_r	6.52e2 nN nm^{-1}
K_θ	8.76e-1 nN nm rad^{-2}
K_ϕ	2.78e-1 nN nm rad^{-2}

nanocomposite. For the purpose of verification, we use the results of reference[31] obtained based on a full MD simulation. The elastic constants extracted from our two-phase and three-phase RVEs are compared with the MD results. To have a proper comparison, the material selected for the polymer matrix is polymethylmethacrylate (PMMA) similar to the MD simulation. The Young's modulus of this isotropic amorphous polymer is assumed to be 2.5 GPa (compared with an experimental range of between 2.24 and 3.8 GPa). For the PMMA polymer matrix, its Poisson ratio is chosen as 0.35. An armchair SWNT (10) with diameter equals to 1.34 nm is placed in the center of the computational simulation cell.

To describe the interaction between the nanotube and the outer polymer matrix at the level of atoms, Hu et al.[32] performed the molecular mechanics computations to obtain the thickness of the transition layer in a CNT/polymer composite. They implemented the molecular mechanics software CERIUS2 to describe the intramolecular interactions between the nanotubes and polymer chains. Their simulations revealed that after putting the polymer chain closely to the nanotube, the chain automatically starts to surround the nanotube. The results showed that the equilibrium distance between H atoms on the polymer and C atoms on the nanotube ranges from 0.2851 to 0.5445 nm. On the basis of this study, we take the average value of this range as the thickness of the transition layer, i.e., 0.42 nm.

As mentioned before, in this work, a homogeneous isotropic interphase medium is inserted between the SWNT and the polymer matrix. The main assumption is that the mechanical properties of the interphase vary continuously between those of the main phases, i.e., CNT and matrix. In this model, the Young's modulus of the transition layer is considered to vary from 1000 to 2.5 GPa which is that of the CNT and PMMA, respectively. Also, the Poisson's ratio of the transition layer is set to be 0.35. The variation in the Young's modulus of the interphase satisfies the following conditions:

$$\begin{aligned} \tilde{E}_i(r) &= E_f \quad at \quad r = r_f \\ \tilde{E}_i(r) &= E_m \quad at \quad r = r_i \end{aligned} \tag{6}$$

where E_f and E_m denote the elastic modulus of the CNT and matrix, respectively. Also, r_f is the CNT radius and r_i stands for the outer radius of the interphase. There are different mathematical models to implement the variations in the elastic properties of an interphase medium in the literature.[17–19,33] For a system of three phases, Saber-Samandari and Afaghi-Khatibi have recently suggested that the modulus of the interphase at any radius r can be calculated from[17,23]:

TABLE II
Input Data for Finite Element Analysis of CNT/PMMA Composite

E_f (GPa)	1000
E_m (GPa)	2.5
E_i (GPa)	93.67[a]
r_f (nm)	0.85
Interphase thickness (nm)	0.42
r_i (nm)	1.27
n	20
$v_m = v_i$	0.35
Length (nm)	12.19

[a] Calculated using eq. (8).

$$\tilde{E}_i(r) = E_m(r_i/r) + [r_i - r)/(r_i - r_f)]^{\frac{n}{2}}[E_f - E_m(r_i/r_f)] \tag{7}$$

where n is the intragallery enhancement factor and is a dimensionless parameter ranging from 2 to 50, which totally depends on the chemistry and surface treatment of the inclusions. Based on the parametric studies in the earlier works, they purposed that $n = 20$ is the proper value for CNT/polymer composites.[23] The average elastic modulus of the interphase E_i can then be derived from the following equation:

$$E_i = \frac{1}{r_i - r_f}\int_{r_f}^{r_i} \tilde{E}_i(r)dr \tag{8}$$

Up to now, the elastic modulus of the CNT, interphase, and polymer matrix used in this work are defined and listed in Table II. Also, the thickness of the interphase layer is assumed to be 0.42 nm based on the previous molecular mechanics works.[32] The only unknown parameter which is necessary in the modeling of the cubic computational RVE is the dimension of the cross-section of the unit cell. This parameter is dependent on CNT volume fraction in the RVE. The CNT volume fraction (f_{CNT}) is an important variable in determining the composite mechanical properties and is defined by:

$$f_{CNT} = \frac{\pi(R_{CNT} + h_{vdw})^2}{A_{cell}} \tag{9}$$

where h_{vdw} is the equilibrium van der Waals separation distance between the CNT and the matrix, and A_{Cell} is the cross-sectional area of the unit cell transverse to the nanotube axis. The van der Waals separation distance depends on the nature of the CNT/polymer interfacial interactions and is assumed to be 0.18 nm in this work in accordance with the earlier works. It is to be noted that atomic scale modeling of a CNT/polymer composite system is rather challenging because of the significant number of atoms

involved, and equilibration times for the polymer that are orders of magnitude longer than a few nanoseconds, which is typically the limit of large classical MD simulations. Thus, the MD simulation work which is referred in this article, has focused on composite systems with a large CNT volume fraction (>10%) to reduce the total size of the model. Considering 12, 17, and 28 percentages for CNT volume fractions in eq. (9), we obtain the cross-sectional dimension of the cubic matrix equals to 4.37, 3.69, and 2.87 nm, respectively. Based on these explanations, geometrical characteristics of the RVEs are as follows:

Armchair nanotube (10, 10): Diameter = 1.34 nm, Length = 12.19 nm
Interphase layer: Thickness = h_{int} = 0.42 nm
Polymer matrix: Length = 12.19 nm, inner radius = $R_{CNT} + h_{vdw} + h_{int}$ = 1.27 nm
Cross-sectional dimension = 4.37, 3.69, and 2.87 nm at different CNT volume fractions.

It is to be noted that the RVE used here is a continuous RVE. Thus, the length of the CNT and the polymer matrix are the same in this work. After constructing the model, the macroscopic behavior of the RVE can be evaluated using the FEM.

RESULTS AND DISCUSSION

Using the introduced three-phase model, a nanocomposite with an armchair (10, 10) CNT, an interphase layer and a PMMA matrix is studied under tensile loading. The main objective is to investigate the effect of interphase on the elastic constants of these nanocomposites, quantitatively. To this end, three-dimensional finite element models including matrix, interphase, and CNT are built to obtain the elastic properties of the polymer matrix nanocomposites. To model the interphase, the CNTs are coated with a thickness of 0.42 nm as the third phase and packed in a cubic matrix. All three phases are completely tied together. In this case, the RVEs of our FEM model are schematically shown in Figure 2. The input data including constituent properties are listed in Table II. Tensile load is applied via a prescribed displacement (0.2 nm) at the longitudinal direction on different RVEs. After determining the properties of the nanotube and the interaction between the nanotube and the polymer matrix, the material properties of the nanotube reinforced composites can be predicted. The elastic modulus of the nanocomposite unit cell, E, is calculated as follows:

$$E = \frac{\sigma}{\varepsilon} = \frac{\frac{F}{A_{cell}}}{\frac{\Delta H}{H_0}} \quad (10)$$

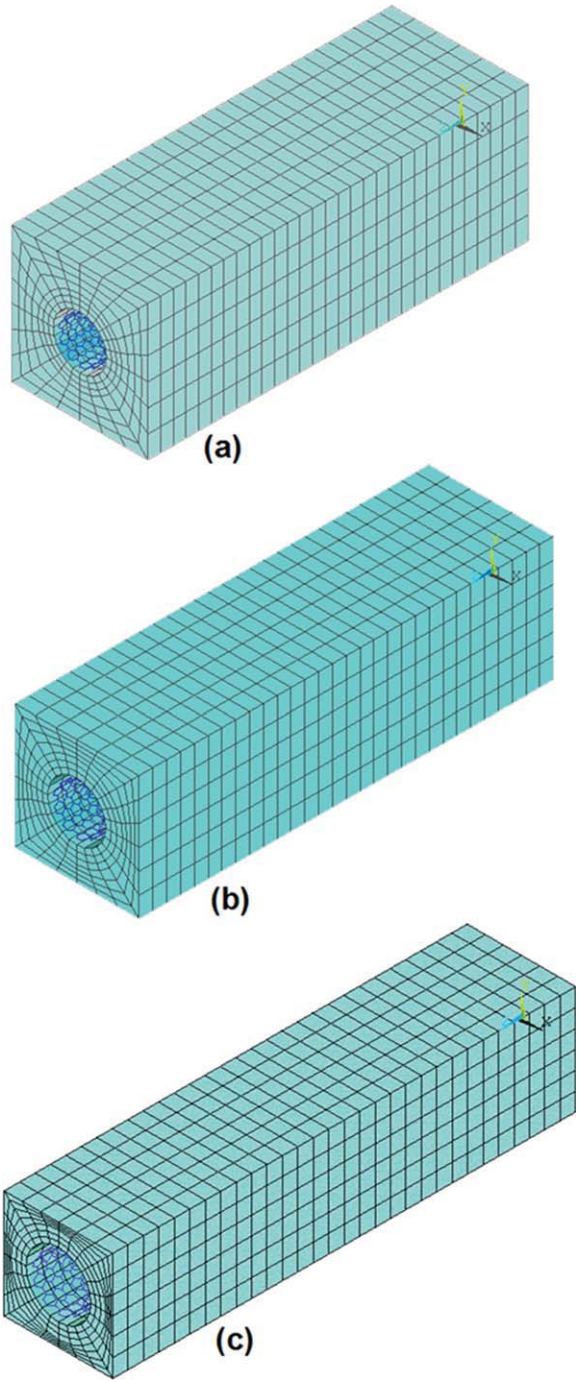

Figure 2 FE macroscopic models of three-phase RVEs at different CNT volume fractions: (a) 12%, (b) 17%, and (c) 28%. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

In eq. (10), F stands for the total force acting at the end of the RVE, H_0 is the RVE initial length and ΔH is its elongation. The units of length and force are nanometer (nm) and nanoNewton (nN), respectively. Thus, the stress and elastic modulus are expressed in GPa.

At the first stage, the Young's modulus of the CNT/polymer computational unit cell has been

TABLE III
Numerical Results for Young's Modulus of CNT/PMMA Composites in GPa

		2-Phase Model		3-Phase Model (This Work)	
f_{CNT} (%)	MD[31]	Results	Deviation from MD	Results	Deviation from MD
12	94.6	81.2	14.2%	92.9	1.8%
17	138.9	114.0	17.9%	137.9	0.7%
28	224.2	186.1	17.0%	225.4	0.5%

calculated without considering the interphase. In the previous sessions, the geometrical and mechanical characteristics of the constituents were introduced. In this study, three unit cells with different CNT volume fractions (12, 17, and 28%) are considered. The results given in Table III show that without considering the interphase, the elastic constants of these nanocomposites have a minimum deviation of 14.2% with the MD results.[31] At the next stage, to investigate the effect of interphase, the Young's modulus is recalculated with the three-phase model involving CNT, interphase, and polymer matrix. The elastic moduli of the nanocomposites with different CNT volume fractions estimated by the new model are compared with the MD results in Table III. As it can be seen from this table, predictions from the new three-phase model are in good agreement with MD results with a maximum deviation of 1.8%. Meanwhile, the computational cost in this method is really negligible in comparison with the MD simulation. These results are also depicted in Figure 3. The results reveal that the interphase properties play a significant role in the stiffness of nanocomposites and the interfacial effects cannot be ignored when interactions between the nanotube and polymer matrix are strong.

In addition, the results obtained by the new three-phase multiscale model, show that increase in the CNT volume fractions has a strong effect on the Young's modulus of CNT/polymer composites. Previous experimental studies and computational modeling techniques, confirm our results.[28,29]

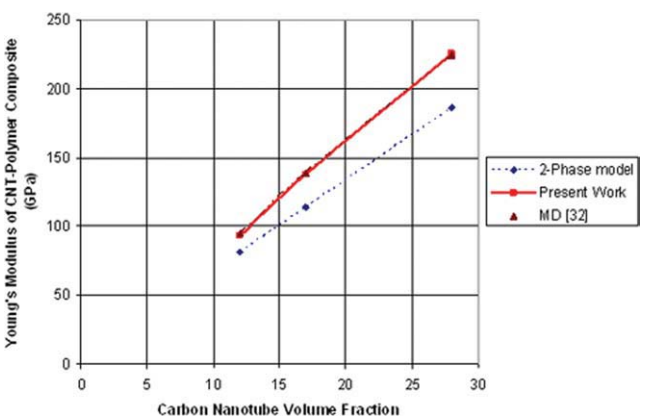

Figure 3 Comparison of the two-phase and three-phase models with MD. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

CONCLUSIONS

In this article, using the molecular structural mechanics approach and the finite element method, the computational modeling of continuous CNT-reinforced polymeric matrix composites has been carried out. To this end, new three-phase multiscale model including CNT, interphase, and matrix is introduced and implemented to evaluate the effect of the interphase on the Young's modulus of CNT/polymer composites. The new model was validated using the results of a standard constant stress MD simulation. In this way, we could investigate the strong role of the interphase layer quantitatively, which had not been considered in the previous similar approaches. Using this model, we showed that increasing the CNT volume fraction in both two- and three-phase models has a strong effect on the Young's modulus of CNT/polymer composites. Also, the results revealed that without considering the effect of the interphase layer, there is a noticeable deviation from the MD results more than 15%. This value, decreases to less than 1.8% after using the interphase as the third phase between the CNT and the polymer matrix. Meanwhile, use of the new three-phase multiscale model, significantly reduces the computational costs in comparison with the MD simulation.

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