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A Continuum-Based Finite Element Model of Carbon Nanotube Polymeric Composite

Saud Aldajah* • **Ammar Al-Omari** • **Yousef Haik**

Mechanical Engineering Department, United Arab Emirates University, Al-Ain, UAE, P. O. Box 17555, United Arab Emirates

Corresponding author: * **s.aldajah@uaeu.ac.ae**

ABSTRACT

The development of a finite element model that is appropriate for the computation of the mechanical properties of nanocomposite materials is the purpose of this research paper. The nanocomposite considered in this research is made of a polymer and aligned carbon nanotubes (CNTs); the applied tensile load is in the same direction of the aligned CNTs. The model development is based on the assumption that carbon nanotubes can be modeled as beam elements using ABAQUS software package. A representative volume element (RVE) method was employed in which it was assumed that the nanocomposite has geometric periodicity with respect to local length scale and that the elastic properties of nanocomposite can be represented by those of the representative volume element. The effective modulus of elasticity predicted by this method is compared with analytical and experimental results available in the literature.

Keywords: carbon nanotubes, FEM, nanocomposite

INTRODUCTION

Composites materials have seen a significant increase in use and have created a revolution in high-performance structures. They exploit the properties of different materials to create structures that are stronger, stiffer, impact resistant and more durable against environmental factors. They can be tailored to have better electric, magnetic, optical properties, and be chemically, thermally and explosion resistant depending on the application. On the other hand, the essence of nanotechnology is the ability to work at a scale of about 1 to 100 nm, in order to create, manipulate, and use materials, devices, and systems that have novel properties and functions because of the small scale of their structures. The nanometer scale is expected to be highly efficient for designing and creating materials, devices and structures with unique properties and functions that traditional chemistry could not create. Also, nanoreinforcement of engineering materials can impart dramatic structural (e.g. stiffness) and physical property benefits without adding significant weight.

A critical issue for nanotechnology is the ability to understand, model, and simulate the behavior of the small structures and to make the connection between structure properties and their functions. Most nano-systems are too small for direct measurements but too large to be described by current rigorous first principles in theoretical physics and computational methods. They exhibit too many fluctuations to be treated monolithically in time and space, and too few to be described by a statistical ensemble. The vital role of modeling in this field is to enable engineering design, at the component and systems level, to set the objectives that could guide laboratory efforts at physical implementation.

Carbon nanotubes (CNT) have become a primary focus in nanotechnology research due to their exceptionally high stiffness and strength. CNT has outstanding Young's modulus and tensile strength and is one of the most promising materials with potential as an ultimate reinforcing material in the nanocomposites (Thostenson *et al.* 2001; Lau *et al.* 2002; Bhushan 2004). Previous studies on the mechanical properties of the CNT show that it has quite broad variation of the Young's modulus ranging from 200 to 4 TPa, tensile strength from 10 to 200 GPa, and bending strength of about 20 GPa (Wagner *et al.* 1998; Li *et al.* 2000; Yu *et al.* 2000; Lau *et al.* 2004). One of the fundamental issues scientists are confronting is the characterization of individual CNTs. Many experimental and theoretical studies have been performed on single and multiple-walled nanotubes (SWCNT and MWCNT). In particular, deformation modes and overall tube stiffness have been closely examined (Zhang *et al.* 2002). However, as materials always fail at the weakest point, it is imperative to examine the performance of nanocomposites as a system, in addition to the structures of nanoparticles. This problem of modeling nanocomposites as a system is highly challenging as CNTs are randomly dispersed in a polymeric (i.e. epoxy) matrix. Thus, physically well grounded, simplified methods for modeling, which can capture significant properties of nano-structured materials, must be developed.

Materials modeling and simulation helps to understand and control materials structure, properties, and processes. Traditionally material behavior is determined through experimental observation. Careful measurements of observed data are subsequently used for the development of models that predict the observed behavior under the corresponding conditions. The models are required to develop the theory. The theory is then used to compare predicted behavior to experiments via simulation. This comparison serves to either validate the theory, or to provide a feedback loop to improve the theory using modeling data. Therefore, the development of a realistic theory of describing the structure and behavior of materials is highly dependent on accurate modeling and simulation techniques. Today's computing power is proving invaluable in the research behind the miniaturization. Computer molecular modeling and simulation is being used to advance the exciting and cutting edge scientific field of nanotechnology, enabling scientists to visualize and predict behavior at the nanoscale (Zhu *et al.* 2007). In this manuscript, we review current procedures used for simulating one of the most famous nano-structured materials i.e., polymer-CNT composites. This includes modeling and simulation of nanocomposites constituents (fiber, mat-

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Research Note

rix and interface). The following are different approaches that can be used to model the nano-structured polymer composites and characterize its effectiveness when the CNTs are aligned within the polymer phase:

Molecular mechanics

An important component in molecular mechanics calculations of the nano-structure of a material is the description of the forces between individual atoms which are characterrized by a force field. The total potential energy of the force field for a nano-structured material is described by the sum of many individual energy contributions:

$$E^m = E^p + E^o + E^T + E^w + E^{vdW} + E^{el} \quad (1)$$

where E^p, E^o, E^T *and* E^w are the energies associated with bond stretching, angle variation, torsion, and inversion, respectively (Xia and Wei *et al.* 2010). The non-bond interaction energies consist of van der Waals, E^{vdW}, and electrostatic, E^{el}, terms. Various functional forms may be used for these energy terms depending on the particular material and loading conditions. Obtaining accurate parameters for a force field amounts to fitting a set of experimental or calculated data to the assumed functional forms (the force constants and equilibrium structure). These constants will be evaluated in the proposed research using published experimental data. Alternatively quantum mechanical calculations may be used to evaluate the force field.

Continuum models of CNTs

In order to simplify the calculation of the total molecular potential energy of molecular models with complex molecular structures and loading conditions, an intermediate model may be used to substitute for the molecular model. This is due to the fact that the MD simulation technique requires long simulation time in order to provide accurate results, however in practice, simulation times are limited. Many researchers modeled CNTs using structural analysis models of truss elements, beam elements. In both cases, the continuum model considered neglected all thermal, quantum and electromagnetic effects. Whereas, for macroscopic structures, the material properties and element sectional parameters can be easily obtained from material data handbooks and calculations based on element sectional dimensions, for nanoscopic CNTs, there is no information about the elastic and sectional properties of the carbon-carbon bonds and material properties. Therefore, it is imperative to establish a link between the microscopic computational chemistry and macroscopic structure mechanics.

In general, the equivalent-continuum model is defined as a continuum that has the following characteristics:

1. Truss lattices, beam elements are modeled as classical continua where micropolar continuum assumptions are not necessary.
2. Local deformations are accounted for the temperature distribution, loading and boundary conditions of the continuum model simulate those of the truss model.
3. The same amount of thermoelastic strain energy is stored in the two models when deformed by identical static loading conditions.

Finite Element Modeling (FEM) can be used for numerical computation of bulk properties based on the geometry, properties, and volume fraction of constituent phases (Dvorak *et al.* 1973). FEM involves discretization of a material representative volume element (RVE) into elements for which the elastic solutions lead to determination of stress and strain field. The coarseness of the discretization determines the accuracy of the solution. Nanoscale RVEs of different geometric shapes can be chosen for simulation of mechanical properties (Liu *et al.* 2003). However, high complexity of models, expensive software, and time-consuming simulations limit the utility of this method. FEM-based micromechanics have been used extensively for the prediction of mechanical properties of nanostructured composites. Many researchers have used FEM-based approach to investigate the mechanical properties of nano composites (Liu *et al.* 2003).

In this paper a nanocomposite made of a polymer and aligned nanotubes is considered where the CNTs were modeled as beam elements. A representative volume element (RVE) method is employed where it is assumed that the nanocomposite has geometric periodicity with respect to local length scale and the elastic properties of nanocomposite can be represented by those of the representative volume element. The effective modulus of elasticity predicted by this method is compared with analytical and experimental results available in the literature. The distinctiveness of the proposed model is that it provides a physically well grounded, simplified model, which can capture the mechanical properties of nano-structured materials.

CONTINUUM BASED MODELING

Generally the continuum-based computational modeling techniques include FEM (finite element modeling) and BEM (boundary element modeling). Both approaches do not always supply exact solutions; they can provide very accurate estimates for a wide range of assumptions.

BEM involves solving boundary integral equations for the evaluation of stress and strain fields. This method uses elements only along the boundary, unlike FEM, which involves elements throughout the volume; thus making this method less computationally exhaustive than FEM (Ingber *et al*. 1997). It can be applied from micro to macro scale modeling. It is assumed that a material continuum exists, and therefore, the details of molecular structure and atomic interactions are ignored. The rigid fiber model has been shown to be very effective in estimation of fiber composites. Ingber *et al*. have shown agreement in predicted modulus using continuum based model and analytical results for fiber composites. Liu *et al*. (2003) used a fast multipole method to model CNT composites. They treated CNTs as rigid fibers and the properties were obtained in an analogous manner to a rigid inclusion problem. The estimated modulus was found to be very close to that predicted by MD simulations. They concluded that the continuum based method can be a very useful for first-order approximation of mechanical properties in large-scale modeling of CNT composites.

The proposed FEM model is a continuum based modeling method which assume the existence of continuum for all calculations and generally do not include the chemical interactions between the constituent phases of the composite The FEM involves discretization of a material representative volume element (RVE) into elements for which the elastic solutions lead to determination of stress and strain field. The shape and size of the RVEs determines the accuracy of the solution. However, the smaller the size of the RVE and the more complex the shape is on the expense of the computing time. The size of the RVE in this model is $20 \times 20 \times 100$ nm. The total size of the nanocomposite was $50 \times 20 \times 20$ μm. ABAQUS 6.7 software was utilized to model the nanocomposite part under unidirectional tensile load.

RESULTS AND DISCUSSION

The current finite element model considers nanotubes as beam elements embedded in resin material. It is assumed that the CNTs are homogeneously distributed within the nanocomposite. There are many studies on the prediction of the mechanical properties of CNTs nanocomposites by using the homogenization method with periodic microstructure (Kanit *et al.* 2003; Cluni *et al.* 2004; Yang *et al.* 2004; Peng *et al.* 2005). Most of them are carried out to obtain the effective mechanical properties of composites reinforced by continuous fiber structures such as woven fabrics on the finite element method (FEM) and the boundary element

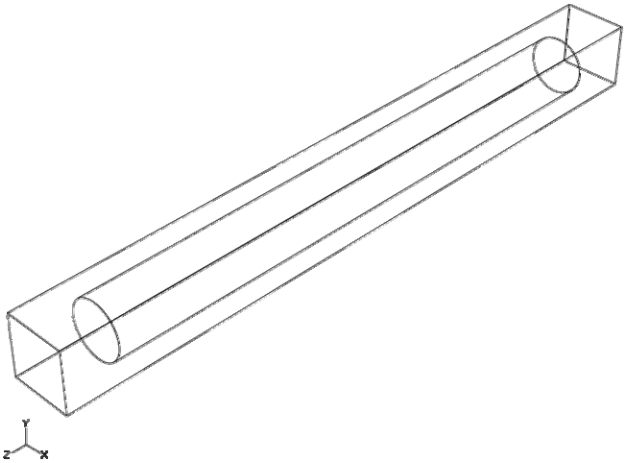

Fig. 1 A representative volume element with a single carbon nanotube in nano scale.

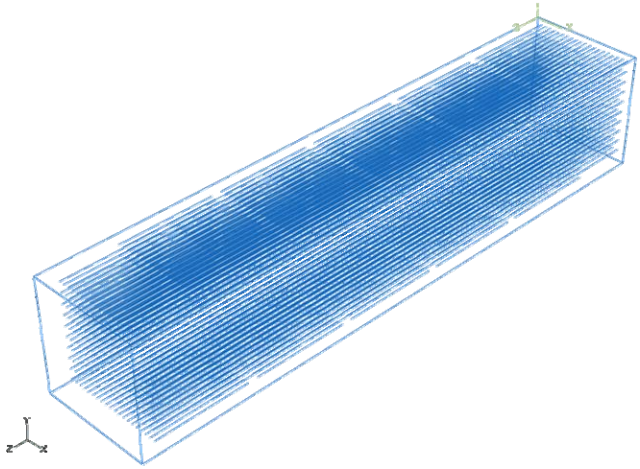

Fig. 2 The representative volume (50 × 20 × 20 µm).

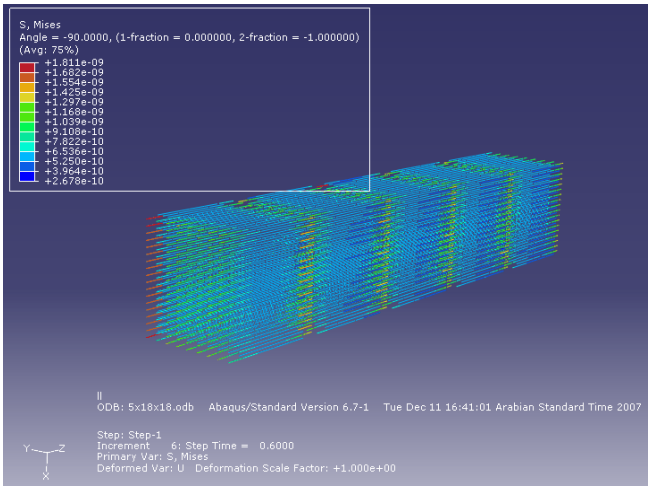

Fig. 3 Nanotube stress distribution.

method (BEM) (Okada *et al.* 2001).

A representative volume was considered as shown in **Fig. 1**. The goal here was to model the effective elasticity tensor for a nanocomposite.

This model simulates the tensile behavior of a 50 × 20 × 20 µm nanocomposite under unidirectional tension, **Fig. 2**. It was assumed that the nanotubes are aligned and are overlapped so that we prevent the ordered sequence which will lead to weak areas resulting in reduced stiffness.

The stress distribution in the nanotubes in the nanocomposite are shown in **Fig. 3** whereas, **Fig. 4** shows the stress

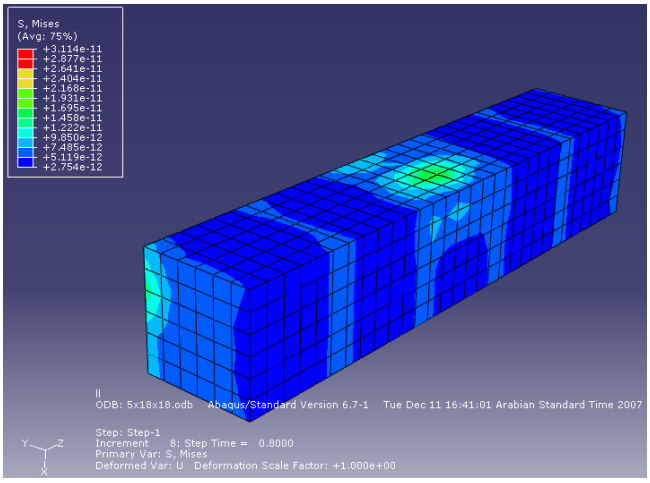

Fig. 4 Nanocomposite stress distribution.

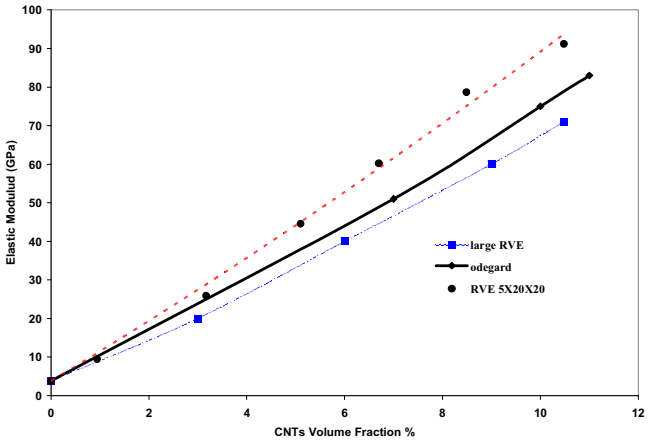

Fig. 5 Elastic modulus vs. CNTs volume fraction percentage.

distribution in the whole nanocomposite. It is possible to calculate the elastic modulus values based on the stress distribution of the nanocomposites as shown in **Fig. 4**. Various nanocomposites models with different CNT volume fractions, namely 1.5, 3, 6, 9 and 11%, were constructed from which the elastic modulus was calculated. After plotting the results of the above models and comparing them with experimental and theoretical data published by Odegard *et al.* (2001), it can be seen that the results of the FEM models are comparable to the published results, **Fig. 5**.

These results are significant due to the fact that the modeling of nano-scale materials is possible using traditional machines. A more accurate approach requires more sophisticated software and computer machines. However, it is possible to further improve the current FEM results by utilizing a smaller RVE which will be the expense of the running computing time and requires more powerful computers.

CONCLUSIONS

Due to the development of nanocomposites and their increased utilization in many engineering applications, it is becoming very important to understand their mechanical behavior through modeling and simulation. Many techniques have been recently developed which include the computational chemistry modeling technique such as the Ab Initio and the molecular dynamics techniques, and the computational mechanics techniques which include the analytical and modeling techniques such as the FEM and BEM techniques. The proposed finite element model is a simplified well grounded model that considers the nanotubes as beam elements embedded in the resin material. The ap-

proach adopted in this model was to discretize the model into smaller parts called RVEs based on the assumption that the CNT/epoxy nanocomposites have geometrical periodicity with respect to the microscopic scale. The constructed model was exposed to a tensile load from which the effective elastic modulus for the nanocomposite was calculated. Different models with different CNT volume fractions were constructed and the overall results were compared to experimental and analytical results available in the literature such as the ones obtained by Odegard *et al.* (2001). The current model results were in good agreement with the analytical and experimental results.

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