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Numerical characterization of CNT-based polymer composites considering interface effects

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ABSTRACT

Carbon nanotubes (CNTs) possess exceptional mechanical properties and are therefore suitable candidates for use as reinforcements in composite materials. Load transfer in nanocomposite materials is achieved through the CNT/matrix interface. Thus, to determine nanocomposite mechanical properties, the interface behavior must be determined. In this investigation, finite element method is used to investigate the effects of interface strength on effective CNT-based composite mechanical properties. Nanocomposite mechanical properties are evaluated using a 3D nanoscale representative volume element (RVE). A single nanotube and the surrounding polymer matrix are modeled. Two cases of perfect bonding and an elastic interface are considered. For the perfect bonding interface, the no slip conditions are applied. To better investigate the elastic interface behavior, two models are proposed for this type of interface. The first elastic interface model consists of a thin layer of an elastic material surrounding the CNT. In the second elastic interface model, a series of spring elements are used as the nanotube/matrix interface. The results of numerical models indicate the importance of adequate interface bonding for a more effective strengthening of polymer matrix by CNT's.

1. Introduction

Since the discovery of carbon nanotubes, CNTs, many investigators have reported remarkable physical and mechanical properties for these fibers [1–5]. The reported density of a SWCNT is about 1.33–1.40 g/cm^3, which is one-half the density of aluminum. The elastic modulus of Single walled carbon nanotubes, SWCNT, is about 1.2 TPa, comparable to that of diamond [6]. The reported tensile strength of SWCNT is as high as 2 GPa which is much higher than that of high-strength steel.

To harness the potential strengthening of nanotubes in manufacturing of nanocomposites, we need to fully understand the load transfer mechanisms between the matrix and the CNTs. The strength of nanocomposite materials is influenced by this load transfer mechanism and the interface strength. Mechanical properties of SWCNT and MWCNTs have been extensively studied both analytically and experimentally [7–10]. Experimental results, however, show large variations in nanotube strength data. Li and Chou determined shear modulus as a function of SWCNT diameter using the molecular structural mechanics approach. Hernandez et al. [11] investigated nanotube diameter dependence of axial modulus using molecular dynamics. Bonora and Ruggiero developed a unit cell model for Metal Matrix Composites (MMCs) and used their model to predict the macroscopic response of SiC/Ti unidirectional composite laminates [12]. Xu and Sengupta [13] used finite element method to investigate the interfacial stress transfer and possible stress singularities in a nanocomposite. Valavala and Odegard presented a review article discussing the major modeling tools available for predicting mechanical properties of nanostructured materials [14]. Liu et al. developed a new continuum model of the CNT-based composites for large-scale analysis at the micro-scale in order to characterize such composites [15]. Chen et al. [16] proposed a micromechanical method to predict the size-dependent plastic property for composite materials. Chen and Liu [17] evaluated effective mechanical properties of CNT-based composites using a square representative volume element (RVE) based on the continuum mechanics using finite element method. Xu et al. performed different mechanical tests to characterize the properties of a new functionalized nanofiber/epoxy composite [18]. Rio et al. [19] prepared nanocomposites with small contents of SWCNT and determined their mechanical properties experimentally. Guz et al. presented a review article discussing application of a number of macro-, meso-, and micromechanical models to nanomaterials [20]. Bogdanivich and Bradford [21] produced macroscopic textile preforms using

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CNTs and used them as reinforcements in making nanocomposite tensile test samples. Thostenson and Chou used a calendaring approach to disperse MWCNTs in epoxy matrix [22]. Kim et al. [23] modified carbon/epoxy composites with carbon nanotubes and investigated the effects of sonication energy on CNT dispersion. Perez and Aviles investigated the influence of interphase thickness on elastic properties of carbon nanotube composites [24].

In the present investigation, the effective mechanical properties of CNT-based composites are determined using a 3D nanoscale representative volume element and FEM. Two types of interface material behaviors are considered, namely: perfect bonding, and an elastic interface. In addition, the elastic interface is modeled using two different approaches as will be discussed in the following section. The RVE model consists of a single nanotube in a surrounding matrix material in both cases.

2. Analysis

The load transfer mechanism at the nanotube/resin interface is investigated in order to determine nanocomposite effective mechanical properties. A square representative volume element proposed by Chen and Liu [17] is used to model the nanocomposite. Two cases of perfect bonding and elastic interfaces are modeled. In the perfect bonding case, a complete load transfer, or no slip, condition is assumed at the interface. In the case of elastic interface, two approaches are taken. First, a thin layer of an elastic material is used as the interface. The effects of bond strength at the CNT/matrix interface on nanocomposite properties are investigated by changing the elastic modulus of this interface layer. Next, a series of spring elements are used on the perimeter of the nanotube to account for the elastic interface. By changing the spring stiffness, the effects of interface strength on nanocomposite mechanical properties are investigated. In this investigation, homogeneous boundary conditions are applied to the RVE models. This is only valid when normal tractions are applied on the boundaries. For shear loading cases, these boundary conditions are over-constrained boundary conditions [25]. The analysis approach is presented in this section.

To derive the relations for extracting the equivalent material constants, a homogenized elasticity model of the square RVE shown in Fig. 1 is considered. The orientation of the coordinate axes is also shown in this figure. A quarter of the RVE is modeled due to symmetry.

Elasticity solutions can be obtained under certain load cases [17]. The RVE consists of a single, transversely isotropic material that has five independent material constants. The four effective material constants namely: Young's moduli E_x and E_z, and Poisson's ratios υ_{xy} and υ_{zx}, are determined in the current investigation. The general 3D strain–stress relations relating the normal stresses and strains for a transversely isotropic material can be written as [17]:

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \end{Bmatrix} = \begin{bmatrix} \frac{1}{E_x} & -\frac{\nu_{xy}}{E_x} & -\frac{\nu_{zx}}{E_z} \\ -\frac{\nu_{xy}}{E_x} & \frac{1}{E_x} & -\frac{\nu_{zx}}{E_z} \\ -\frac{\nu_{zx}}{E_z} & -\frac{\nu_{zx}}{E_z} & \frac{1}{E_z} \end{bmatrix} \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{Bmatrix} \quad (1)$$

To determine the four unknown material constants (E_x, E_z, υ_{xy} and υ_{zx}), four equations are needed. Two different loading cases, illustrated in Fig. 2a and b, have been devised to provide these equations based on the elasticity theory [17]. In the first loading case, shown in Fig. 2a, the RVE is subjected to a known axial elongation. In the second loading case, shown in Fig. 2b, the RVE is subjected to a known lateral distributed load. A two-dimensional view of Fig. 2b indicating the symmetry boundary conditions is shown in Fig. 3. Formulations for each of these loading cases are presented in the following sections.

2.1. Square RVE under an axial elongation

In this case, the stress and strain components on the lateral surface are given by;

$$\sigma_x = \sigma_y = 0,\ \varepsilon_z = \frac{\Delta L}{L},\ \varepsilon_x = \frac{\Delta x}{a} \text{ along } x = \pm a, \quad \text{and;}$$

$$\varepsilon_y = \frac{\Delta y}{a} \text{ along } y = \pm a$$

where Δa is the change of the cross section length, a, under the elongation ΔL in the z-direction. Integrating and averaging the third equation in (1) on the plane $z = L/2$, we obtain

$$E_z = \frac{\sigma_{ave}}{\varepsilon_z} = \frac{L}{\Delta L}\sigma_{ave} \quad (2)$$

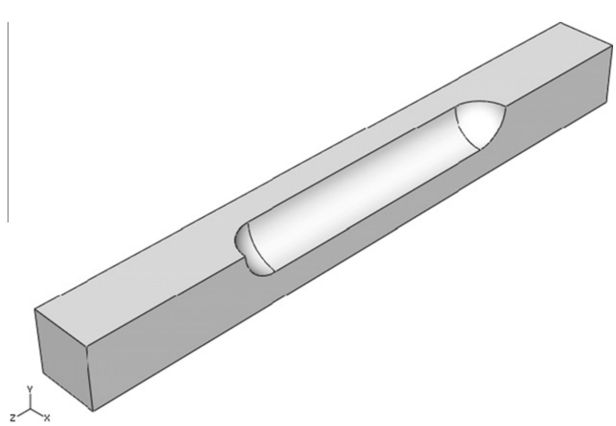

Fig. 1. Quarter of the RVE used to model the CNT-based polymer composite.

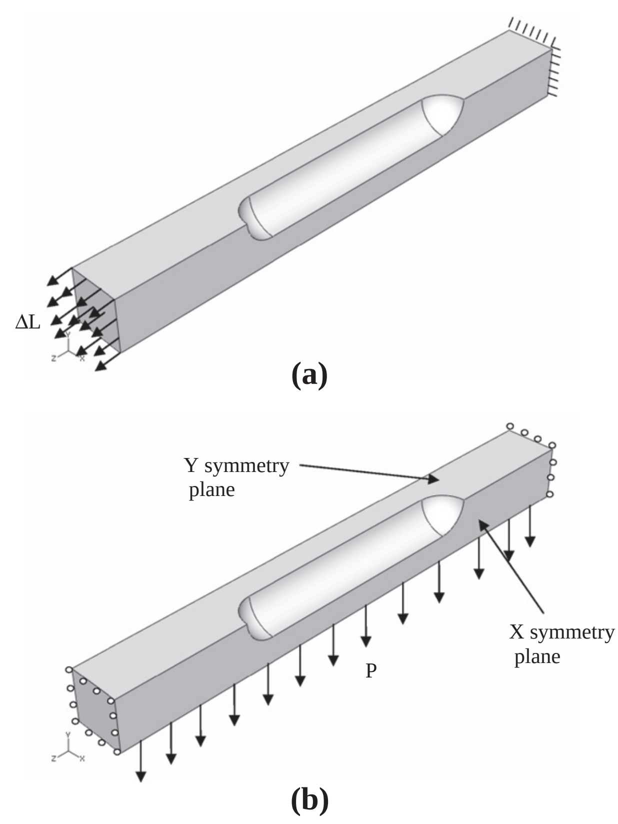

Fig. 2. The loading cases: (a) RVE under an axial elongation ΔL, (b) RVE under a transverse distributed load P.