Composites: Part B 56 (2014) 100–108

Contents lists available at ScienceDirect

Composites: Part B

journal homepage: www.elsevier.com/locate/compositesb

Mechanical property characterization of carbon nanotube modified polymeric nanocomposites by computer modeling

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ARTICLE INFO

Article history:
Received 28 May 2013
Accepted 12 August 2013
Available online 22 August 2013

Keywords:
A. Polymer-matrix composites (PMCs)
B. Mechanical properties
C. Finite element analysis (FEA)
C. Statistical properties/methods

ABSTRACT

This paper reports a two-step modeling approach for predicting the effective mechanical properties of polymeric nanocomposites modified with single walled carbon nanotube (SWNT). In step one, the nano-heterostructures of the nanocomposites were represented by 3-D nanoscale cylindrical, square, or hexagonal prismatic representative volume elements (RVEs). Each RVE contained a long or a short carbon nanotube (CNT) and consisted of three phases, i.e., CNT, matrix, and interphase. The mechanical properties of each RVE were extracted from the modeling results of the RVE undergone three load tests, i.e., uniaxial tensile test, lateral expansion test, and axial torsional test, using appropriately derived formulae. The effects of the volume fraction of CNTs on the mechanical properties of the RVEs were studied. The equivalent mechanical properties of the nano-heterostructures were obtained by averaging the mechanical properties extracted from each RVE. In step two, micro/macroscale nanocomposites were represented by a 3-D microscale unit cell which was discretized into cubic elements. Using Monte Carlo method, each element was assigned the averaged mechanical properties of the RVEs with random CNT orientation and length type. The overall effective mechanical properties of the nanocomposites were predicted by a tensile test on the unit cell. The modeling results by this proposed approach was compared with and validated by the experimental data of the SWNT modified epoxy nanocomposites.

1. Introduction

Since being discovered by Iijima [1], carbon nanotubes (CNTs) have drawn much attention due to their high flexibility, strength, and stiffness, as well as superior electrical and thermal properties. Numerous studies have been performed to determine the mechanical properties of this nano-structured material [2–14]. Theoretical and experimental investigation indicated an average Young's modulus of around 1 TPa and Poisson's ratio of 0.25–0.28 for single-walled carbon nanotubes (SWNTs), depending on the CNTs' length, diameter, chirality, sample synthesis, type of defect, measurement techniques, and computational theory and parameters.

Nanocomposites are composite materials in which the matrix material is reinforced by nanomaterials in order to modulate its properties. Carbon nanofibers and nanotubes are promising to revolutionize several fields in material science and are one of the major components of nanocomposites [15–20]. Tensile tests on the composite films showed that 1 wt% of CNTs added in the polymer matrix resulted in 36–42% and ~25% increases in elastic modulus and break stress, respectively [21]. However, CNT's potential for reinforcement of polymers has not been fully realized.

A composite has three phases – matrix, fiber and interphase between these two. At the micro or larger scale, the size and effect of the interphase might be negligible. However, in nanocomposites, the interphase could play important role [22–25]. Recently, computer modeling of the mechanical properties of CNTs/polymer nanocomposites based on a three-phase model has been done by using molecular dynamics (MD) simulation [26–31] and finite element analysis (FEA) [22–25,32–35]. The results confirmed that the interphase had significant effects on the performance of a nanocomposite material. The MD simulation approach is limited to very short length and time scales and cannot deal with large scale in nanocomposites due to the limitation of computing power (for example, a $1 \times 1 \times 1\ \mu m^3$ cube could contain up to 10^{12} atoms). As nanocomposites varying from nanoscale to microscale, continuum approach based on continuum mechanics has to be considered.

To address the difficulties in obtaining the equivalent properties of the nano-heterostructures, a concept of nano-scale representative volume elements (RVEs) was introduced. RVE refers to a sample of the material that structurally has the entire characteristics of the mixture on the average, typically represented by a cylindrical,

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1359-8368/$ - see front matter
http://dx.doi.org/10.1016/j.compositesb.2013.08.052

square, or hexagonal prismatic bar containing one CNT. Otherwise, it must be statistically representative of the micro/macro response satisfying statistical homogeneity and ergodicity of the material. In reality, nanocomposites are not homogeneous continua but rather heterogeneous and random media, where the CNTs are not periodic and/or uniform in the structure. In this case the quality of the derived results depends strictly on the size of the material region chosen and the orientation and distribution of the RVEs/CNTs.

The physical properties of the materials with nano-heterostructures depend on the production and fabrication procedures. Changes in the factors such as orientation and volume fraction of fillers (CNTs), process temperature, pressure and time, voids, and impurities, induce variations in the effective (or overall, microscopic or macroscopic) material constitutive properties. The scatter and uncertainty in the material structure and properties are considered as random, i.e., the randomness in geometry, orientation and dispersion of inclusions in the base material. Effective use of reinforced polymeric nanocomposites and design of reliable products rely upon an accurate characterization of the inherent random nature of a heterogeneous nano/micro structure in the materials. Therefore, the necessity of establishing statistical and probabilistic based models is evident [36–42].

In this paper, a two-step modeling of the mechanical properties of SWNT modified polymeric nanocomposites is proposed, as shown in Fig. 1. In the first step, three types of nanoscale RVEs (cylindrical, square, and hexagonal) containing a long or a short CNT were designed. Each RVE included three phases: fiber, matrix, and interphase. Uniaxial tensile, lateral expansion and axial torsion tests on each RVE were designed and conducted by computer modeling. The formulae based on elasticity theory were derived for extracting the equivalent mechanical properties (Young's moduli and Poisson's ratios) from the modeling results of the RVEs undergone these three load tests. The effect of the volume fraction of the CNTs was studied. The mechanical properties extracted from the RVEs were averaged and compared with the rule of mixture analysis. In the second step, in order to predict the effective mechanical properties of a macro/microscale nanocomposites, a 3-D microscale nanocomposite unit cell was discretized into cubic elements, and the averaged mechanical properties of the RVEs from the step one were input into each element taking into account the randomness of the CNT's length type and orientation using Monte Carlo method. The overall effective mechanical properties of the unit cell were predicted from a tensile test using FEA. The computer modeling results of the CNT reinforced epoxy nanocomposites were compared with the experimental data.

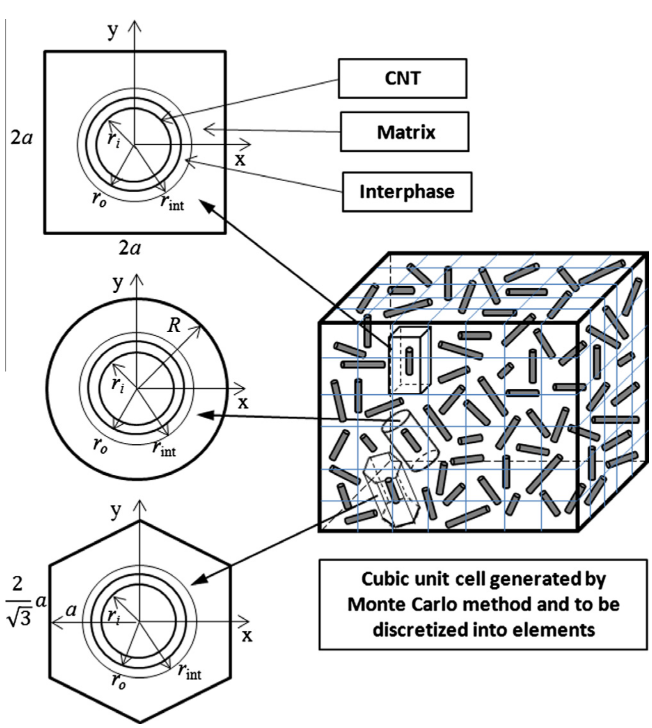

Fig. 1. Schematic representation of three types of RVEs (cylindrical, square, and hexagonal) that consist of three-phases (polymer matrix, CNT filler, and interphase), and a statistical model of a unit cell generated by Monte Carlo method. Each RVE includes a short or long CNT.

2. Mechanical property formulations for RVEs

Three types of nanoscale RVEs, i.e., cylindrical, square, and hexagonal prismatic bars, are designed. To derive the formulae for extracting the equivalent material constants, homogenized prismatic solid elasticity models, having the same outer dimensions as for the RVEs and filled with a single and transversely isotropic material are used. In the RVEs, the CNTs, the matrix and the interphase are considered as continua, being of linear elastic, isotropic and homogeneous materials with specific Young's moduli and Poisson's ratios. It is further assumed that the CNTs and the matrix have perfectly bonded interface in the RVE. Each RVE contains only one short or long CNT aligned along the RVE length direction. Since the formation of a CNT with end caps reduces the total surface energy, the model of the short CNT with hemispherical end caps is adopted. Under the above assumptions, four effective material constants (Young's moduli $E_x(=E_y)$ and E_z, and Poisson's ratios ν_{xy} and $\nu_{zx}(=\nu_{zy})$, which are related to the normal stress and strain components) will be determined for the CNT-based composite. The 3-D normal stress–strain relationship for a transversely isotropic material can be written as

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

The effective material constants (E_x, E_z, ν_{xy}, and ν_{zx}) can be determined by uniaxial tensile, lateral expansion, and axial torsion tests on the RVEs.

2.1. Cylindrical RVE

Firstly, the RVE is undergone a uniaxial tension ΔL, resulting in an average lateral contraction of ΔR_a ($\Delta R_a < 0$), as shown in Fig. 2(a). Therefore,

$$E_z = \frac{\sigma_z}{\varepsilon_z} = \frac{L}{\Delta L}\bar{\sigma}_z \tag{2}$$

where the axial average stress $\bar{\sigma}_z$ can be calculated by averaging the FEA results.

$$\bar{\sigma}_z = \frac{1}{A}\int_A \sigma_z\left(x, y, \frac{L}{2}\right)dxdy \tag{3}$$

with A being the cross-sectional area. Similarly, the Poisson's ratio, ν_{zx}, can be calculated as,

$$\nu_{zx} = -\left(\frac{\Delta R_a}{R}\right) \Big/ \left(\frac{\Delta L}{L}\right) \tag{4}$$

Then, the RVE is undergone a lateral uniform expansion by a negative pressure p and constrained in the z-direction at both ends