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Micromechanical modeling of nanocomposites considering debonding and waviness of reinforcements

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ABSTRACT

This paper deals with a constitutive model of carbon nanotube (CNT)-reinforced composites which describe the debonding damage and waviness effects of reinforcements on mechanical properties of nanocomposites simultaneously. It is observed that the lack of fiber waviness distribution and weak bonding assumption lead to inaccurate composite stiffness prediction. Based on the present model, analysis of stress–strain response for CNT/polymer composites under uniaxial tension is carried out. At constant strains while considering interfacial debonding of inclusions, CNT-reinforced composites with more curved CNTs have additional area under the curve and therefore accomplish higher toughness. In presence of poor bonding, CNT waviness can enhance the composite stiffness rather than reducing it. A quite different conclusion with respect to what can be obtained with the assumption of perfect bonding. Moreover, the waviness and interfacial debonding of inclusions have effect on Poisson's ratio of CNT-reinforced nanocomposites. The Poisson's ratio decreases first then it increases by increasing the waviness parameter.

1. Introduction

The high strength and stiffness of carbon nanotubes have generated enormous interest in the scientific community in recent years [1]. In fact, the unique atomic structure, high aspect ratio, light weight, extraordinary mechanical properties, and thermal conductivity make carbon nanotube (CNT) a potentially very promising candidate as the ideal reinforcing fibers for advanced composites with high strength and low density [2].

In CNT-reinforced nanocomposites, the elastic modulus and the strength are improved significantly over that of the matrix with only a very small fraction of the CNTs [3,4]. On the other hand, it is also widely recognized that the experimental mechanical properties of CNT-reinforced nanocomposites are quite different from the theoretical expectation [5–7]. It is shown that the unsatisfactory improvement in the mechanical properties of CNT-reinforced composites could be attributed to the weak bonding between CNTs and polymer matrices [6,8–10] as well as the waviness and agglomeration effects of CNTs [7,9–11]. Since the weak CNT–polymer interface, poor CNT dispersion and waviness effect of CNTs can weaken considerably the thermal, electrical and mechanical properties of the composites. Thus, it is important to determine the effect of these defects on the effective properties of CNT/polymer composites.

Due to the huge difference between the stiffness and strengths of the CNTs and most of the matrix materials and the complicated mechanisms at the interface, weak bonding areas are quite likely to exist, and debonding may occur at very low level of loading or even during manufacturing. Thus the assumption of perfect bonding between CNTs and surrounding resin which is treated in micromechanics rules is not correct and weak bonding is a critical factor that decides the reinforcing efficiency of the CNTs. Moreover, the micrograph images [11–13] show that the embedded CNTs remain highly curved when dispersed in a polymer matrix. The waviness of CNTs is a key factor that influences the reinforcing efficiency of CNTs and weakens the capability of CNTs as reinforcement in comparison with straight CNTs [14–19]. In the majority of previous studies, the effect of waviness on the effective properties of CNT/polymer composites is investigated by assuming a sinusoidal waviness.

Damage modes are thought to depend on the combination of the mechanical properties of the constituents and in situ interfacial strength. Among them in the nanocomposites, the fracture of reinforcements and the interfacial debonding are the major damage modes, so that two modes mainly affect the mechanical performance of the nanocomposites. Therefore to extend the application of the nanocomposites and to develop even a new

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composite, thorough understanding of the micromechanics of damage process is essential. In this paper, the effects of the curvature and interfacial debonding of reinforcements in the carbon nanotube-reinforced polymer composites are analyzed simultaneously. The wavy CNTs are replaced by equivalent straight short fibers in both vertical and horizontal projection. The developed incremental constitutive law predicts the effective properties of the nanocomposite while considering the debonding process. Accordingly, the aim of this work is to present a micromechanically-based model while simultaneously considering the waviness and debonding of the reinforcements in the CNT/polymer composites.

The stress–strain response under uniaxial tension is carried out on CNT-reinforced nanocomposites and the influence of the debonding and waviness of reinforcements on stress–strain curve is discussed. Moreover, in this work the effect of debonding and waviness of the reinforcements on the effective Young's modulus and Poisson's ratio of CNT-reinforced nanocomposites is demonstrated. To validate the predictions of the proposed model, the results are compared to those obtained from the experimental results presented by Andrews et al. [20] and Villoria and Miravete [21]. The proposed model and the experimental results are shown to be in good agreements.

2. Modeling procedure

2.1. Micromechanical model for curved CNTs

Experimental observations and micrograph images show that the embedded CNTs remain highly curved when dispersed in a polymer [8,11,17]. In this investigation the model that considered analyzing the waviness effect of CNTs in the polymer matrix is the one proposed by [7]. In this model, the CNTs is considered as solid short fibers with a circular cross-section exhibiting bow shape waviness, as shown in Fig. 1. It is obvious that a curved CNT will have reinforcing effects both in the chord and in perpendicular directions. Therefore, in order to simulate the reinforcing effect of a curved CNT in a composite, it is projected onto the vertical and horizontal directions, respectively.

Here a and λ are the amplitude (vertical projection) and half-wavelength (horizontal projection) of a curved CNT, respectively. $\delta = \frac{a}{\lambda}$ is introduced as a parameter which shows the effect of waviness. By using this model, the curved fiber is replaced by one straight fiber along the chord, and two other straight fibers in the perpendicular direction. In the first step, volume fraction of equivalent fiber in the chord and perpendicular direction should be evaluated.

The volume fraction of the CNTs, υ_f can be defined as [7]

$$\upsilon_f = \upsilon_2 + \upsilon_3, \quad \upsilon_2 = \frac{N\pi d^2 \lambda}{4V}, \quad \upsilon_3 = 2\frac{N\pi d^2 a}{4V} \tag{1}$$

where υ_2 and υ_3 are volume fraction of fiber in the chord and perpendicular direction, respectively.

N is the number of CNTs, d is the diameter of the CNTs, and V is a representative volume of a CNT/polymer composite.

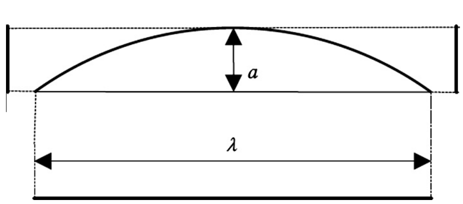

Fig. 1. The model of a curved CNT.

From Eq. (1), the relation between υ_2 and υ_3 can be defined as follows:

$$\frac{\upsilon_2}{\upsilon_3} = \frac{1}{2\delta} \tag{2}$$

From Eqs. (1) and (2), υ_2 and υ_3 can be rewritten based on waviness parameter δ as follows:

$$\upsilon_2 = \frac{\upsilon_f}{1+2\delta}, \quad \upsilon_3 = \frac{\upsilon_f}{1+1/2\delta} \tag{3}$$

In the next step, the effective modulus of the vertically and horizontally projected equivalent fiber should be calculated. The effective modulus of the horizontally projected fiber, E_{υ_2}, and the effective modulus of the vertically projected fiber, E_{υ_3}, are obtained from the rule-of-mixture as below

$$E_{\upsilon_2} = \frac{E_x - E_m \upsilon_m}{\upsilon_2}, \quad E_{\upsilon_3} = \frac{E_y - E_m \upsilon_m}{2\upsilon_3} \tag{4}$$

where E_m is Young's modulus of the SMP matrix and υ_m is the volume fraction of the matrix. E_x and E_y are the effective modulus of a composite which contains straight uniaxial fibers in chord and perpendicular directions, respectively.

Here, the results of the effective longitudinal and transverse moduli in Refs. [22,23] are adopted, as follows:

$$\begin{aligned} E_x &= \frac{(1+c)^{3/2}}{(1+\frac{c}{2})S_{11} - \left[1+\frac{3c}{2}-(1+c)^{3/2}\right]S_{22} + \frac{c}{2}(2S_{12}+S_{66})} \\ E_y &= \frac{(1+c)^{3/2}}{\left[1+\frac{3c}{2}-(1+c)^{3/2}\right]S_{11} - (1+\frac{c}{2})S_{22} + \frac{c}{2}(2S_{12}+S_{66})} \end{aligned} \tag{5}$$

where

$$c = \left(\frac{\pi a}{\lambda}\right)^2, \quad S_{11} = \frac{1}{E_L}; \quad S_{22} = \frac{1}{E_T}, \quad S_{12} = -\frac{\upsilon_{LT}}{E_L}; \quad S_{66} = \frac{1}{G_{LT}} \tag{6}$$

In the above formulas, E_L, E_T and G_{LT} are the longitudinal, transverse and shear moduli of the composite with the uniaxial straight fibers. υ_{LT} is the longitudinal–transverse Poisson's ratio. Substituting Eqs. (5) and (6) into Eq. (4), the effective moduli of the horizontally and vertically projected equivalent fiber can be obtained.

After the replacement of curved fiber with two kinds of equivalent straight fibers, a stepping scheme is applied to predict the effective properties of composites with several kinds of inclusion [24]. In this method the inclusions are treated step by step and the effective stiffness coefficients are calculated for the resulting composite in each step. The main idea of stepping scheme of multi-inclusion problem can be described as follows. Firstly, add one kind of inclusion to the matrix material and make a homogenization of the current composite. Then take the current composite as a new matrix and add another kind of inclusion to the new matrix. The homogenization is carried out. Such a process will be repeated for all kinds of inclusions. The effective properties obtained by the final homogenization are the macroscopic properties of multi-inclusion composite.

To considering the interfacial debonding effect of reinforcements, the incremental damage theory is applied for each step.

2.2. Incremental damage theory

In Fig. 2, the states of the composite before and after incremental deformation in the damage process are depicted. The state before incremental deformation shown in Fig. 2a is described in terms of the volume fractions of the intact and damaged reinforcements f_p and f_d. If the volume fraction of the inclusions that are debonded during the incremental deformation is denoted by df_p, then the state after deformation, shown in Fig. 2b, can be described