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A new micromechanics model and effective elastic modulus of nanotube reinforced composites

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ABSTRACT

In the present study, a new model, in which the wavy carbon nanotubes are replaced with effective fibers, has been developed. The analytical expressions are derived based on the micromechanics method, then the effective elastic modulus of carbon nanotube (CNT)/polymer composites can be predicted. This paper mainly investigates the effects of waviness and agglomeration on the effective elastic modulus of curved carbon nanotube reinforced composites. It is found that both of those factors can significantly affect the stiffening of composites. The stiffness of carbon nanotubes can be reduced significantly due to the effects of waviness and agglomeration. Moreover, the effects of waviness and agglomeration on the effective elastic modulus are also discussed. It is noted that the effective elastic modulus of CNT reinforced composites is very sensitive to the waviness and the agglomeration.

1. Introduction

To-date, the remarkable properties of carbon nanotube (CNT) attract much attention of scholars. Many investigators have reported its unique properties, and especially the CNT can be considered as one of the most promising reinforcements for composites. It is shown that the elastic properties and tensile strength of epoxies increased 200% and 140% only attending with 0.5 wt% single wall carbon nanotubes (SWCNTs) [1,2]. There are many ways in studying the effects of CNT on mechanical properties of CNT-reinforced composites [3–7]. In all of the approaches, however, the effective fiber is an important bridge. It is noted that the CNT is a non-continuous structure in a nanoscale, and the traditional micromechanics can't be used to analyze it directly. Therefore, the different types of effective fibers should be proposed. Odegard et al. [8] proposed an effective continuum fiber which links atomistic simulations of nano-structured materials to continuum models of corresponding bulk materials.

Shady and Gowayed [9] and Shi et al. [10] investigated the effect of waviness on effective modulus of composite, and in their studies the CNT was assumed as a special helical shape. The strain energies of nanotube and effective fiber were estimated, and moreover, the effective elastic modulus of composites was also predicted. Shady and Gowayed [9] thought that the effect of curvature seems more critical with increase of weight fraction. However, Shi et al. [10] got that the waviness has little effect on the lateral modulus. Giannopoulos et al. [11] employed a cylindrical representative, which consists of the reinforcement, the interface and the matrix material. This study gives a micromechanical finite element approach for the estimation of the effective Young's modulus of nanotube reinforced composite.

Based on the finite element method, researchers [12,13] found that an increase in the amount of randomness results in decreased Young's modulus values and strength of composite. Investigations [14,15] consider the wavy nanotube following an infinitely long sinusoidal shape. Here, the effective modulus of material with aligned or randomly oriented inclusions was obtained based on a Mori–Tanaka model. As a result, the waviness reduces the elastic modulus in the nanotube direction of a polymer reinforced with oriented wavy nanotubes, as compared to only straight nanotubes [14–16].

The aim of the present paper is to investigate the effective elastic modulus of carbon nanotube (CNT)/polymer composites, with emphasis on the influence of CNT waviness and agglomeration on the composite. A new model replacing the wavy carbon nanotubes with effective fibers has been developed. The effect of waviness and agglomeration on the effective elastic modulus of composites is mainly investigated using a Mori–Tanaka method. Analytical expressions are also derived for predicting the effective elastic modulus of carbon nanotube reinforced composites. It is shown that both of these factors, i.e., waviness and agglomeration can significantly affect the stiffening effect on composites. Moreover, it is also found that the effective moduli obtained are very sensitive to the waviness and agglomeration of carbon nanotubes.

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2. Theoretical formula for curved CNTs reinforced composites

2.1. Micromechanics model for curved CNTs

Based on the experimental results and micrograph images [13,14,17–19], the CNTs generally exist in a wavy shape in nanocomposites (refer to Fig. 1). For a simplification, Shao et al. [17] first proposed that the nanotubes are treat as solid short fibers with a circular cross-section and exhibit a bow shape waviness, as shown in Fig. 1. Here a and λ are the amplitude (vertical projection) and wavelength (horizontal projection) of the spatial wavy fiber. The diameter and volume fraction of CNTs are denoted by d and f_r. It is obvious that a spatial wavy fiber will have reinforcing effects in the both directions of axis and perpendicular to the axis, as shown in Fig. 2. Then, the spatial wavy fiber is replaced by a straight fiber along the axis and two other straight fibers in the perpendicular direction as shown in Fig. 3. Therefore, the volume fractions of equivalent fiber in the axis and perpendicular direction should be evaluated at first.

The volume fraction of CNTs can be defined as follow,

$$f_2 = N\frac{\pi d^2 \lambda}{4V}, \quad f_3 = 2\cdot N\frac{\pi d^2 a}{4V} \tag{1}$$

where f_2 and f_3 are volume fractions in the chord and perpendicular direction, respectively. N is the number of CNTs, d is diameter of the CNTs and V is a representative volume of a CNT-reinforced composite.

$$\text{So, we have} \quad f_2 + f_3 = f_r \tag{2}$$

From Eqs. (1) and (2), introducing a parameter $\delta = \frac{a}{\lambda}$ which shows the effect of waviness, we get

$$\frac{f_2}{f_3} = \frac{1}{2\delta}, \quad f_2 = \frac{f_r}{1+2\delta}, \quad f_3 = \frac{f_r}{1/2\delta + 1} \tag{3}$$

In the next step, we need calculate the effective modulus of an equivalent fiber. It is assumed that the effective modulus of a spatial CNT is provided by the straight fiber. Through the rules-of-mixtures, we get as belows:

$$E_{f2}f_2 + E_m f_m = E_x, \quad 2E_{f3}f_3 + E_m f_m = E_y \tag{4}$$

where E_{f2} and E_{f3} are the effective moduli of horizontally projected fiber and vertically projected fiber, respectively, E_m is Young's modulus of the polymer matrix. E_x and E_y are the effective longitudinal and transverse modulus of a composite.

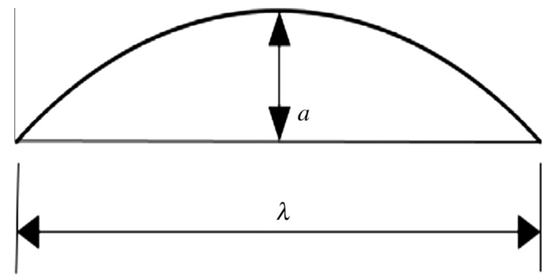

Fig. 2. The model of a curved CNT.

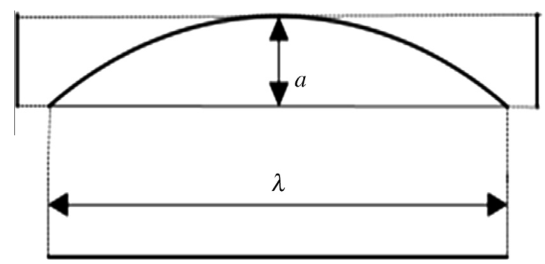

Fig. 3. The projection of a curved CNT.

It should be noted that there have been some studies predicting the effective modulus of composites reinforced by continuous curved fibers [20,21]. Here, we adopt the results of effective longitudinal and transverse modulus [20,21] as follows:

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

$$E_y = \frac{(1+c)^{3/2}}{\left[(1+c)^{3/2} - 1 - \frac{3c}{2}\right]S_{11} + (1+\frac{c}{2})S_{22} + \frac{c}{2}(2S_{12}+S_{66})} \tag{6}$$

where

$$c = \left(\frac{\pi a}{\lambda}\right)^2 = \pi^2\delta^2 \tag{7}$$

$$\left.\begin{array}{l} S_{11} = \frac{1}{E_1};\ S_{22} = \frac{1}{E_2} \\ S_{12} = -\frac{\nu_{12}}{E_1};\ S_{66} = \frac{1}{G_{12}} \end{array}\right\} \tag{8}$$

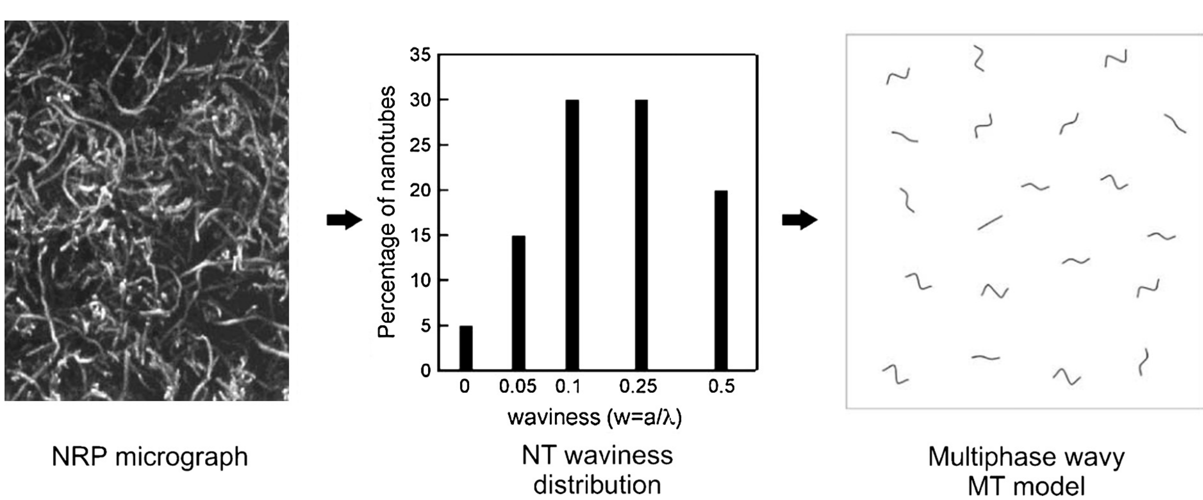

Fig. 1. Model of CNTs reinforced polymer composites with a known waviness distribution function.