A Study on Effective Elastic Modulus of Nanocomposites

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Abstract. Nanocomposites reinforced by carbon nanotubes exhibit great advantages in engineering applications. The waviness of nanotubes is one of the important factors which affect the effective elastic modulus of nanocomposites. This paper aims to develop a new model to replace the wavy carbon nanotubes with effective fiber. The effective modulus of nanocomposites with randomly oriented fibers can be predicted based on the micromechanics. The effects of waviness and agglomeration on the effective modulus are also analyzed. It is shown that they can reduce the stiffness of carbon nanotubes, significantly. Moreover, the effective elastic modulus of nanocomposites is very sensitive to the waviness and the agglomeration.

Introduction

To-date, many researchers have studied on the effective elastic modulus of nanocomposites. From the discovery of carbon nanotube (CNT), its remarkable properties attract much attention of scholars [1-3]. Many effects, e.g., CNT geometry and dispersion, ratio of length and diameter, and interfacial bonding on mechanical properties of CNT-reinforced composites have been investigated in some ways [4-6]. Shady and Gowayed [7] investigated the effect of waviness on effective modulus of composite based on the fact assuming the CNT as a special helical shape. It has been found that the effect of curvature seems more critical with increasing weight fraction. Moreover, the strain energy of nanotube and the effective fiber are predicted, and the constraints imposed by the matrix on the deformation are considered in this study.

As compared with an experimental analysis, numerical method is often employed as an effective way for the mechanical behavior of nanocomposites, since it cost less and doesn't need to establish complex evaluation. Giannopoulos et al. [8] gives a micromechanical finite element approach for the estimation of effective Young's modulus. In the work of Giannopoulos et al. [8], a cylindrical representative, which consists of reinforcement, interface and matrix material is employed, and a discrete spring-based finite element method is used to simulate the nanotubes. Based on the finite element method, it has been found that an increase in the amount of randomness results in decreased Young's modulus values and strength of composite [9].

The aim of present paper is to investigate the effective elastic modulus of CNT-reinforced composites. We will pay more attention to the influence of CNT waviness and agglomeration on the composite. A spatial wavy fiber with a solid circular cross-section is used to simulate the actual CNT state in the matrix. Then, we replace the spatial wavy fiber with a straight fiber along the axis and a coin shape wafer. Both fiber and coin shape are assumed to be isotropic, and then the effective modulus can be determined by the Mori-Tanaka effective-field method propose.

Micromechanics Model

Many experimental results have shown that CNTs generally exist in a wavy shape in the nanocomposites. In this study, parameters a and λ are the amplitude and wavelength of spatial wavy fiber. The diameter and volume fraction of CNTs are denoted by d and f_r . Then, we replace the

spatial wavy fiber with a straight fiber along the axis and a coin shape wafer. The length and the volume fraction of straight fiber are denoted by λ and f_1 . The radius, the volume fraction, and the thickness of wafers are denoted by a , f_2 and h , respectively.

Considering a representative volume V of a CNT-reinforced composite, we have the relations:

$$f_1 = N \frac{\pi d^2 \lambda}{4V} \quad (1)$$

$$f_2 = N \frac{\pi a^2 h}{4V} \quad (2)$$

$$h = \frac{d^2}{a} \quad (3)$$

where N is the number of a certain CNTs with same waviness which is identified by the ratio a/λ denoted by δ . From Eqs. 1, 2, and 3, we can obtain:

$$\frac{f_1}{f_2} = \frac{\lambda}{a} \quad (4)$$

In order to remain the volume fraction, it is assumed that the sum of straight fiber volume and wafer volume equals to the carbon nanotube volumes. Then, we can express this relation as,

$$f_1 + f_2 = f_r \quad (5)$$

Summarizing equations above, we can obtain:

$$f_1 = \frac{f_r}{1 + \delta} \quad (6)$$

$$f_2 = \frac{\delta \cdot f_r}{1 + \delta} \quad (7)$$

It is assumed that the spatial CNT horizontally effective modulus is provided by the straight fiber. Through the rules-of-mixtures, we get

$$f_1 E_1 + f_m E_m = E_x \quad (8)$$

$$f_2 E_2 + f_m E_m = E_y \quad (9)$$

where E_m is the Young's modulus of matrix, f_m and f_1 are the volume fractions of matrix and straight fibers, respectively. Here, we adopt the result of effective longitudinal modulus [10],

$$E_x = \frac{(1+c)^{3/2}}{(1+\frac{c}{2}) \cdot S_{11} - [1+\frac{3c}{2} - (1+c)^{3/2}] \cdot S_{22} + \frac{c}{2} (2S_{12} + S_{66})} \quad (10)$$

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

where

$$c = \left(\frac{2\pi a}{\lambda}\right)^2 = 4\pi^2 \delta^2 \quad (12)$$

$$\begin{aligned} S_{11} &= \frac{1}{E_L}; S_{22} = \frac{1}{E_T} \\ S_{12} &= -\frac{\nu_{LT}}{E_L}; S_{66} = \frac{1}{G_{LT}} \end{aligned} \quad (13)$$

In the above formulas, E_L , E_T , and G_{LT} are the longitudinal, transverse and shear moduli of composite with wavy fibers. Term ν_{LT} is the longitudinal-transverse Poisson's ratio. The rules-of-the mixtures can be used to obtain these parameters,

$$\begin{aligned} E_L &= f_r E_r + f_m E_m \\ E_T &= \left(\frac{f_r}{E_r} + \frac{f_m}{E_m}\right)^{-1} \\ \nu_{LT} &= f_r \nu_r + f_m \nu_m \end{aligned} \quad (14)$$

According the intrinsic relationship, we can get:

$$G_f = \frac{E_f}{2(1+\nu_f)}, G_m = \frac{E_m}{2(1+\nu_m)} \quad (15)$$

From the above analysis we can get the effective elastic modulus of straight and wafer,

$$\begin{aligned} E_1 &= \frac{E_x - f_m E_m}{f_1} \\ E_2 &= \frac{E_y - f_m E_m}{f_2} \end{aligned} \quad (16)$$

Results and Discussion

The respective effective moduli of composites containing curved fibers and corresponding straight fibers are predicted. Note that these two fibers have the same length. To estimate the effective elastic modulus of composite reinforced by both of wavy CNTs and agglomerated CNTs, the effective elastic stiffness of inclusions is calculated and then figure up the overall property of whole composite system. In this study, the parameters used are presented in Table 1.

Table 1. Parameters and ratios used for numerical calculations.

E_m (GPa)	ENT (GPa)	a/λ	λ/d	$\nu_m = \nu_{Nt}$
2.25	450	0.05	60	0.30

The CNTs are divided into concentrated and freely scattered ones in the matrix. The region agglomerated CNTs nearby matrix is assumed to be spherical in shape and the freely scattered ones are thought in a spatial wavy shape as shown in Fig. 1. Then, we replace the spatial wavy shape with a straight fiber and a wafer. So there are three kinds of inclusions in the matrix.

Fig. 1. Inclusion model Proposed for the agglomeration of CNTs.

Fig. 2 gives the variation of effective elastic modulus with the increase of waviness for different volume fractions. It can be found from Fig. 2 that there is almost no obvious influence of waviness on the value of effective elastic modulus when $0 < \delta < 0.1$. However, the effective elastic moduli are very sensitive to the waviness in the region of $0.1 < \delta < 0.3$. Moreover, it's noted that the value of effective elastic modulus seems no longer change much when δ is over 0.3.

Fig. 2. Effective elastic modulus versus waviness for different volume fractions.

Conclusions

In this investigation, based on the micromechanics, a new model to replace the wavy carbon nanotubes with effective fibers has been developed. It can be used to predict the effective elastic modulus of nanocomposites with randomly oriented effective fibers. The effects of both waviness

and agglomeration on the effective elastic modulus are also discussed. As a result, it is found that the stiffness of carbon nanotubes can be reduced, significantly due to the influences of waviness and agglomeration of nanotubes. Moreover, there is a significant influence of waviness and agglomeration on the effective elastic modulus of nanocomposites.

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