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Effective Young's modulus of carbon nanotube/epoxy composites

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ABSTRACT

A formulation based on shear-lag model and global force equilibrium is proposed to identify the effective Young's modulus of single and multi-walled carbon nanotube (CNT)/epoxy composites. The effective Young's modulus from the model is validated by available experimental results and good agreements are identified. The results show that an increase in CNT length, CNT layer number, interspace shear modulus between adjacent CNT layers and CNT volume percentage leads to an increase in the effective Young's modulus. It is found that the effective Young's modulus of a ten-walled CNT/epoxy composite is as high as 152 GPa with the CNT half-length of and CNT volume percentage being 8200 nm and 14.5%, respectively. It also reveals that although a single-walled carbon nanotube (SWCNT) composites have a superior load transfer, the SWCNTs demonstrate a weaker reinforcing capability than its counterparts, multi-walled CNTs.

1. Introduction

Nanoscale reinforcing capability of CNTs in composite industry has been widely studied [1–5] owing to their exceptionally resilient with a remarkably large strength in comparison with the conventional reinforcing fibers, such as carbon fibers. Studies on load transfer in CNT composites are indispensable to improve the strength of CNT composites [6–8]. Studies on Young's modulus of CNT composites and effects of matrix and CNT properties and geometries on the Young's modulus have also been conducted by experiments, theories and computer simulations. Omidi et al. [9] carried out a tensile test to obtain the mechanical properties of multi-walled CNT (MWCNT)/epoxy composites for various weight percentages of MWCNTs. Experimental results show that the Young's modulus and the tensile strength of the composites can be significantly improved by adding a small percentage of MWCNTs. A new form of the rule of mixtures, including an exponential shape function, length efficiency parameter, orientation efficiency factor and a waviness parameter was proposed. Ayatollahi et al. [10] studied the effects of MWCNTs on mechanical properties of epoxy/MWCNT composites in terms of fracture toughness under bending and shear loading. It was also found that the Young's modulus of MWCNT/epoxy composites increases with a rise of MWCNT weight percentage. Liu et al. [11] carried out tensile and nano-indentation tests to find mechanical properties of MWCNT/Nylon-6 composites. Results showed that the elastic modulus and the yield strength of the CNT-reinforced composites are greatly improved by about 214% and 162%, respectively with a CNT weight percentage of 2%. The effect of CNT aspect ratio on the reinforcement efficiency at low filler contents in an epoxy system is experimentally investigated [12]. A theoretical model using the micromechanical approach to predict the elastic modulus of CNT composites was carried out [13]. Results indicate that a larger CNT radius induces a lower effective Young's modulus of CNT composites. Identifying the Young's modulus of composites reinforced by conventional fibers based on the shear-lag model has been also implemented [14,15]. Computer simulations including the molecular dynamics simulations [16,17] and finite element simulations [18] have been carried out to identify the effective Young's modulus of CNT-based composites under tension. The aforementioned approaches to predict the effective Young's modulus of CNT composites are having its own limitations. There are lacks of proper direct measuring techniques at the nanometer scale and not able to control over alignment and waviness of CNT in hosting matrix in experiments [19,20]. The computer simulations are limited and only handled with small model sizes. Theoretical model is able to overcome the limitations faced by experiments and computer simulations. However, the quantity of theoretical studies is

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showing a modesty. One of reasons is that the MWCNT has a complicate nature of the problem involving many CNT layers which bond each other via the van der Waals interactions [21]. As a result, a development of a new theoretical model to identify the effective Young's modulus of composites associated with numerous CNT layer numbers is critical in understanding the potential of CNT composites. Answers to some critical issues by the new model such as the effect of CNT layer numbers, length and volume percentage on the effective Young's modulus of CNT composite are indispensable in applications of CNT-reinforced composites.

In the study, a formulation based on viewpoint of global force equilibrium for the composites are proposed to investigate the effective Young's modulus of CNT/epoxy composites. In this regard, an application of the shear-lag model for 2-D representative element volume (RVE) is presented to evaluate the axial displacements which are then used in the proposed formulation to predict the effective Young's modulus of CNT composites. Based on the proposed formulation, the value of the effective Young's modulus is identified and effects of lengths, layer numbers, and volume percentages of CNTs on the effective Young's modulus are investigated. Without loss of generality, CNT/epoxy composites with CNTs having layer number from 1 to 10 are used in this analysis.

2. Shear-lag model

In order to study the effective Young's modulus of the CNT-reinforced composites, the atomic discrete structure of CNTs is converted into continuum structure, in which the shear-lag model is adopted [22–24]. The variation of stress on the thin CNT layers in transversal direction is negligible and only the stress in the longitudinal direction is focused [7,22]. In this study, the CNTs are assumed to be straight and perfectly aligned with the applied force. The parameters used in the present work are shown in Fig. 1, wherein L, $R_{i.0}$ and $R_{i.1}$ are CNT half-length as well as RVE half-length, outer and inner radii of the epoxy matrix, respectively. The parameter $q = R_{i.0}–R_{i.1}$ represents the thickness of the epoxy matrix in x-direction. The 2-D RVE structure is constructed symmetrically with respect to both x and y coordinate axes. In the study, perfect alignment, perfect dispersion and no waviness of CNTs within epoxy matrix are assumed. Moreover, the perfect bonding between matrix and outermost CNT layer is assumed and used. It also assumes that there is no thickness of this interspace [7,25]. Radii, $R_{i.1}$~$R_{i.2n}$ are the outer and inner radii of CNTs associated with n layers, respectively. In the study, p and s are individual CNT thickness and the gap between two adjacent layers, respectively. The values of p and s are selected based on [26] as shown in Table 1 below. The inner radius of the innermost layer, n, is firmly chosen as $R_{i.2n} = 5\ nm$. Subsequently, the outer and inner radii of CNT layer are $R_{i.2n-1} = R_{i.2n} + + 0.14$ nm and outer and inner radii of the gap between two adjacent layers are defined as $R_{i.2f-2} = R_{i.2f-1} + 0.2\ nm$, where f is the interspace number index. The abovementioned radius relationships are applied to the RVE with n CNT layers. An initial stress denoted as σ_{0m} is only applied to the matrix [7,25]. For simplicity, the 3-D model of the cylindrical RVE is simplified into a 2-D model with all properties of the 3-D model remaining the same in the 2-D model. In the model, the gap between two adjacent layers is also treated as an entity governed by the van der Waals interaction modeled by a modulus [7,22]. Based on the shear-lag model, one infinitesimal element of the layer 2 with a size of dy is considered and examined the force equilibrium on it. Where ε_m, ε_1, ε_2, and ε_3 stand for the axial strains of the matrix and CNT layers 1, 2, and 3, respectively. A three-layered model shown in Fig. 1 can be extended to a model containing a larger layer number. It is noted that the axial stress of the cross-section of the epoxy matrix is a function of x. For simplicity, it is assumed that there is no bonding between the CNT ends and the matrix [7]. In order to facilitate the shear-lag model to calculate the strains, the average of the axial stress in the matrix is defined as $\sigma_{a.m}$ [6,25]:

$$\sigma_{a\cdot m} = \frac{1}{\pi\cdot\left(R_{i\cdot 0}^2 - R_{i\cdot 1}^2\right)} \int_{R_{i\cdot 1}}^{R_{i\cdot 0}} \sigma_m(x,y)\cdot 2\pi\cdot x\cdot dx \tag{1}$$

The equivalent average strain of matrix, $\varepsilon_{a\cdot m}$ can be further obtained as

$$\varepsilon_{a\cdot m} = \frac{1}{\pi\cdot\left(R_{i\cdot 0}^2 - R_{i\cdot 1}^2\right)} \int_{R_{i\cdot 1}}^{R_{i\cdot 0}} \varepsilon_m(x,y)\cdot 2\pi\cdot x\cdot dx \tag{2}$$

In the study, the interspace shear stress governing the facial sliding between two adjacent layers is assumed to be proportional to the difference of two axial strains of the two adjacent layers surrounding it. Hence, the following relation for the interspace shear stress is obtained:

$$\tau_{i\cdot j} = \frac{R_{a\cdot(1,n)}}{s} G_{is^*}\cdot\left(\varepsilon_j - \varepsilon_{j+1}\right) \quad j = 1,2,3\ldots n-1 \tag{3}$$

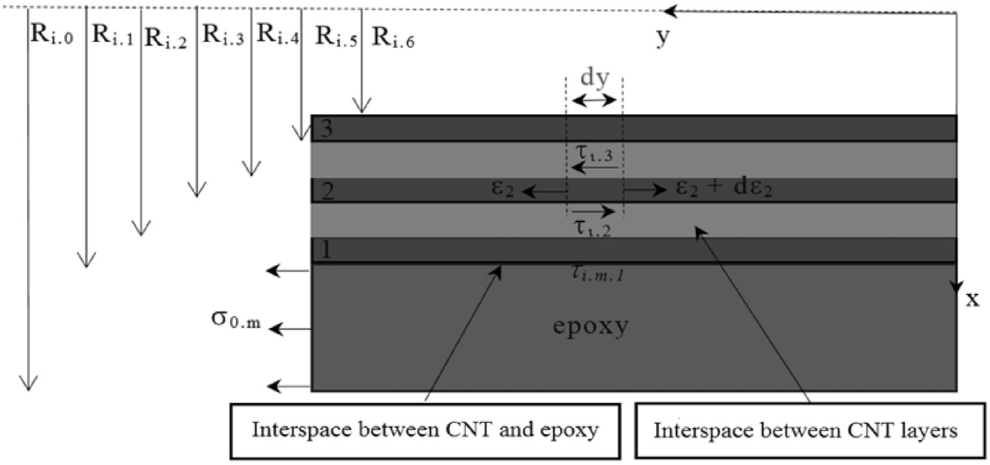

Fig. 1. Shear-lag model for a three-walled CNT-reinforced composite under tension.