ANALYTICAL AND NUMERICAL TECHNIQUES FOR PREDICTING THE INTERFACIAL STRESSES OF WAVY CARBON NANOTUBE/POLYMER COMPOSITES

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By introducing a new simplified 3D representative volume element for wavy carbon nanotubes, an analytical model is developed to study the stress transfer in single-walled carbon nanotube-reinforced polymer composites. Based on the pull-out modeling technique, the effects of waviness, aspect ratio, and Poisson ratio on the axial and interfacial shear stresses are analyzed in detail. The results of the present analytical model are in a good agreement with corresponding results for straight nanotubes.

1. Introduction

Carbon nanotubes (CNTs) have attracted great interest since their discovery in the late 1990s [1] due to their unique electronic and mechanical properties, such as the extremely high elastic modulus (1 TPa), tensile strength, and resistance to failure. A detailed summary of the mechanical properties of CNTs can be found in [2]. The high strength and elastic modulus, the fibrous shape, and the very great aspect ratio of these tubes make them ideal candidates for an ultrastrong reinforcement of composites [3]. These polymer-based nanocomposites usually show remarkable improvements in various physical properties even at a very low content of CNTs, compared with those of virgin polymers or conventional microcomposites.

In the development of nanotube-reinforced polymer composites (NTRPCs), one of the fundamental issues that scientists and engineers are confronting is the nanotube/polymer interfacial bonding, which determines the load transfer capability from the matrix to a nanotube (NT). Hence, the knowledge and understanding of the nature and mechanics of load transfer between the nanotubes and a polymer is critical for manufacturing enhanced NTRPCs. Wagner [4] employed the Kelly–Tyson (KT) model, which has been widely used to study the matrix–fiber stress transfer mechanism in micron-size fiber composites, to examine the interfacial shear strength between an NT and a polymer matrix. Additionally, Lau [5] conducted an analytical study on the interfacial bonding properties of NTRPCs by using the well-developed local density approximation model, the classical elastic shell theory, and the conventional fiber pull-out model; and Gou et al. [6] investigated the molecular interactions between a nanotube and a thermosetting matrix (epoxy resin) during composite processing.

In addition, micrographs show that embedded nanotubes often exhibit a significant curvature (wavy behavior) in a polymer. Jortner [7] have reviewed some of the earliest works on the elastic behavior of wavy fiber composites.

In this paper, an analytical model is developed to investigate the effect of nanotube waviness on the interfacial stress transfer characteristics of SWCNT/polymer composites, which is based on conventional fiber pull-out models. The model is capable of predicting the axial and interfacial shear stresses along a carbon nanotube (CNT) embedded in a matrix. The numerical results obtained show that the waviness of CNTs is very important in governing the interfacial stress transfer characteristics of CNT/polymer composites.

2. Geometric Structure of SWCNTs

Carbon nanotubes are the fourth allotrope of condensed carbon. Two varieties of these tubes are distinguished — single-walled (SWCNTs) and multi-walled carbon nanotubes (MWCNTs).

SWCNTs are generated by rolling up a Graphene sheet into a seamless cylinder with a constant radius. The atomic structure of nanotubes depends on the tube chirality, which is defined by the chiral vector \( C_h \) and the chiral angle \( \theta \). The chiral vector is defined as the line connecting two crystallographically equivalent sites O and C in a two-dimensional Graphene structure, as shown in Fig. 1.

The chiral vector \( C_h \), chiral angle \( \theta \), and diameter \( D \) of CNTs can be defined in terms of the lattice translation indices \((n, m)\) and the basic vectors \( a_1 \) and \( a_2 \) of the hexagonal lattice as follows:

\[
C_h = na_1 + ma_2,
\]

\[
\theta = \sin^{-1} \left[ \frac{\sqrt{3}m}{2\sqrt{m^2 + mn + n^2}} \right],
\]

\[
D = a_0 \sqrt{n^2 + mn + m^2} / \pi,
\]

where \( a_0 = \sqrt{3}a_{c-c} \) and \( a_{c-c} = 0.1421 \) nm. SWCNTs can be further divided into three classes, namely zigzag \((m=0)\), armchair \((m=n)\), and chiral ones, depending on the chiral indices.

3. Analytical Formulation

Despite the discrete nature of the atomic structure of CNTs, we will treat them as having a solid circular cross-section, which introduces two simplifications into the analysis. First, the hollow nature of the NTs is neglected. Second, by modeling the nanotube as a continuum, we disregard any possible relative motion between individual shells or tubes in a MWNT and an
NT bundle. In addition, the individual phase materials are modeled as linear elastic and isotropic. Also, perfect bonding between the polymer and CNTs is assumed.

Consider a wavy NT of solid cross section shown in Fig. 2. The equation describing the NT waviness is

\[ y = A \cos \frac{2\pi z}{\lambda}, \]

where \( \lambda \) and \( A \) are the sinusoidal wavelength and amplitude of the fiber, respectively.

The arc element of the NT can be described as follows:

\[ ds = \frac{dz}{\cos \theta} = \sqrt{1 + 4\pi^2 \left( \frac{A}{\lambda} \right)^2 \sin^2 \frac{2\pi z}{\lambda}} \, dz. \]

Assuming that the NT takes up the pull-out force \( P \), the boundary conditions at the ends of this model are (Fig. 2)

\[ \sigma_{NT}^z (0) = \sigma_{pull-out}, \quad \sigma_{NT}^z (\lambda) = 0, \quad \sigma_m^z (0) = 0, \]

\[ \sigma_m^z (\lambda) = \gamma \sigma_{pull-out}, \quad \sigma_{pull-out} = \frac{P}{A}, \]

where \( \sigma, P, \) and \( A \) are the stress, axial load, and cross-sectional area of the NT, respectively. The subscripts m and NT refer to the materials of the NT and matrix, respectively; \( \gamma \) is the area ratio of the NT and matrix, i.e.,

\[ \gamma = \frac{A_{NT}}{A_m} = \frac{D^2}{B^2 - D^2}, \]

where \( D \) and \( B \) are diameters of the NT and matrix, respectively.

Employing equilibrium equations, boundary conditions, and the continuity at the bonded interfaces, solutions for the stress distribution can be obtained from the differential equation

\[ \frac{d^2 \sigma_{NT}^z (z)}{dz^2} - A_1 \sigma_{NT}^z (z) - A_2 \sigma_{pull-out} = 0. \] (1)

The quantities \( A_1 \) and \( A_2 \) are functions of the mechanical properties and geometrical factors of the nanotube and matrix:
\[ A_1 = \frac{(1 - 2K\nu_{NT})}{U_2 - 2KU_1}, \quad A_2 = \frac{-\gamma(1 - 2K\nu_m)}{U_2 - 2KU_1}. \]

Designating by \( E_{NT}, \nu_{NT} \) and \( E_m, \nu_m \) the elastic moduli and Poisson ratios of the NT and polymer matrix, respectively, we have

\[ U_1 = \frac{\gamma}{8} \left\{ \frac{\eta_1}{2} B^2 \ln\left(\frac{D}{B}\right) \left[ 1 + \gamma \left(\frac{B^2 - D^2}{2}\right) \right] - \gamma \frac{\eta_2}{2} \left(\frac{B^2 - D^2}{2}\right) \right\}, \]

\[ U_2 = \frac{\gamma \nu_m}{4} \left[ \frac{\eta_1}{2} B^2 \ln\left(\frac{D}{B}\right) \left(1 + \gamma \right) \frac{\eta_2}{2} \left(\frac{B^2 - D^2}{2}\right) \right] \]

\[ K = \frac{\alpha \nu_{NT} + \gamma \nu_m}{\alpha(1 - \nu_{NT}) + 1 + 2\gamma + \nu_m}, \quad \alpha = \frac{E_{NT}}{E_m}, \quad \eta_1 = \frac{2(1 + \nu_m)}{\nu_m}, \quad \eta_2 = \frac{(1 + 2\nu_m)}{\nu_m}. \]

The magnitudes of the axial and shear stresses are highly affected by the properties and geometrical factors of the NT and matrix. It should be mentioned that, for straight NTs \((a = 0)\), Eq. (1) is reduced to a differential equation reported earlier in [5, 8].

The equilibrium equations for the stresses can be expressed as (see Fig. 3):

\[ \sigma_{NT}^z \pi D^2/4 - (\sigma_{NT}^z + d\sigma_{NT}^z) \pi D^2/4 - \tau \pi D ds = 0 \Rightarrow \frac{d\sigma_{NT}^z}{ds} = -\frac{4}{D} \tau, \]

\[ \sigma_m^z \pi B^2/4 - (\sigma_m^z + d\sigma_m^z) \pi B^2/4 + \gamma \pi B ds = 0 \Rightarrow \frac{d\sigma_m^z}{ds} = \frac{4\gamma}{B} \tau. \]

4. Numerical Results

In this section, numerical examples are given for CNT/polymer composite systems to demonstrate the distribution of axial and interfacial shear stresses of the wavy CNTs in a fully bonded region. The material properties and geometrical characteristics of the CNTs and matrix are as follows [9]:

\[ D = 5 \text{ nm}, B = 1 \mu\text{m}, \nu_m = 0.48, \nu_{NT} = 0.3, E_m = 3 \text{ GPa}, E_{NT} = 900 \text{ GPa}, A/\lambda = 0.1, P = 20 \text{ nN}, \lambda = 1 \mu\text{m}. \]
Fig. 4. Normalized axial $\sigma/\sigma_{\text{pull-out}}$ (a) and interfacial shear $\tau/\sigma_{\text{pull-out}}$ (b) stresses vs. the normalized coordinate $z/\lambda$ at $A/\lambda = 0$ (---), 0.1 (---), 0.2 (---), and 0.3 (---).

Fig. 5. Normalized axial $\sigma/\sigma_{\text{pull-out}}$ (a) and interfacial shear $\tau/\sigma_{\text{pull-out}}$ (b) stresses vs. the normalized coordinate $z/\lambda$. For (a) --- $\lambda/D$, $A/\lambda = (100, 0)$ (---), (100, 0.1) (---), (200, 0) (---), and (200, 0.1) (---); for (b) $\lambda/D = 200$ (---), 100 (---), and 50 (---).

Fig. 6. Effect of Poisson ratio $v_m$ on the axial (a) and interfacial shear (b) stresses of NRPCs: $v_m = 0.3$ (---), 0.4 (---), and 0.48 (---).
Figure 4 shows variations in the normalized axial $\sigma/\sigma_{\text{pull-out}}$ and interfacial shear $\tau/\sigma_{\text{pull-out}}$ stresses in NRPCs along the dimensionless axial coordinate $z/\lambda$ for different values of NT waviness. As seen, the maximum interfacial shear stress occurs at $A/\lambda$ and increases gradually as the waviness increases. Also, the average axial stress of the wavy NT is lower than that of straight ones. The results for straight CNTs $A/\lambda = 0$ are in a good agreement with published data [5].

According to Fig. 5, with increasing wavelength of the NT, the maximum interfacial shear stress increases, but the axial stress drops sharply to zero.

From Fig. 6, it is obvious that the Poisson ratio has a negligible effect on the interfacial shear stress for both straight [8] and wavy NTs.

5. Conclusions

Based on the pull-out modeling technique, a new simplified 3D representative volume element for wavy CNTs has been developed to study the effect of their waviness, aspect ratio, and Poisson ratio on the axial and interfacial shear stresses of NRPCs. The results of calculations led to the following conclusions:

- the maximum interfacial shear stress of wavy NTs is higher than that of straight ones and increases with increasing waviness, but the variation trend of the average axial stress is reverse;
- with increasing wavelength of NTs, the maximum interfacial shear stress increases;
- as in the case of straight NTs, the effect of Poisson ratio on the interfacial stresses of wavy NTs can be ignored;
- the model proposed can also be utilized in an analysis of other problems for nanotube-reinforced polymers, including the viscoelastic response and the thermal and electrical conductivity;
- the correlation between the results from the analytical model and those for straight NTs is very satisfactory.

REFERENCES