AN INTERFACE MODEL OF THE FIBER PULLOUT PROCESS OF THE CARBON NANOTUBES (CNT) HYBRIDIZED CARBON FIBER (HCF) COMPOSITES

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Keywords: Hybrid composites, Interface shear strength, Finite element analysis with user subroutine, Nano composite

Abstract

In this paper, An interface model of the hybridized carbon fiber composites is proposed for analyzing fiber pullout process. HCF means CNTs hybridized on the carbon fiber surface by Chemical Vapor Deposition (CVD). Compared to the prevalent three-phase analysis model, this model combines the CNT pullout theory and the cohesive zone model (CZM),which is employed to represent microscale influence of CNT pullout. This model is verified by the results of single fiber pullout test. Compared to untreated carbon fiber/matrix, numerical results show that interfacial shear strength of HCF/matrix interface is improved by the addition of CNTs. In the parametric study, we consider the influence of morphology of CNTs in HCF pullout problem. The numerical results illustrate interfacial shear strength can be improved with the increasement of the distribution density and aspect ratio of CNTs.

1. Introduction

Recently，the novel CNT reinforced composites, HCF composite as shown in **Figure 1**[1] have significant potential to expand the performance and functionality of fiber-reinforced composites. HCF composite demonstrated a widely advantage behavior including enhancement in bolt-bearing strength, thermal conductivity[2] and electrical conductivity[3]. Especially, some experiments demonstrate an excellent interface shear strength between the CNT hybridized carbon fiber and the polymer matrix. An et al.[4] prepared the multiscale carbon nanotube-hybridized carbon fiber by a newly developed aerosol-assisted chemical vapor deposition method, discussed fracture models along with fiber pulling out from epoxy composites and demonstrated a 94% increasement in the interfacial shear strength.

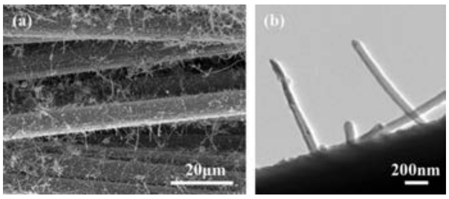

Figure 1.carbon nanotubes reinforced with carbon fiber by the CVD method(Copyright © 2013 Elsevier Ltd)[1]

Compared to the experimental research, theoretical and numerical analysis can provide additional insight into the reinforcing effect of CNTs for the nano composites and assist the further development and optimization design of composites. Kundalwal et al.[5] used a three-phase shear lag model to analyze the stress transfer characteristics of the short fuzzy fiber reinforced composite incorporating the staggering effect of the adjacent representative volume elements. Ray[6] used a novel three-phase

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shear lag model to study the load transfer characteristics of the short fuzzy fiber reinforced composite subjected to the thermo-mechanical loading. Curtin[7] developed a shear-lag model for a ceramic matrix composites containing wavy, finite-length and statistical distribution of strengths nanofibers. Wang et al.[8] calculated the pullout force–displacement relation of short fibers grafted with CNTs which reflects the fracture model of the CNTs as found in the experiments[4].

In numerical studies, Prabhat et al.[9] studied the effect of CNT length and density on the interfacial properties of HCF composites by CZM. The parameters of CZM are obtained from the experimental results which restrained the application of this model. Jia et al.[10] simulated the multiscale CNT/CF hybrid fiber pullout using the spring elements. Romanov et al.[11] developed a 3D FE model to predict stress distribution in a unidirectional fiber composite reinforced with CNTs. Ren et al.[12] use a 3D computational multiscale mechanical-electrostatic coupled model in order to study the piezoresistive response of fuzzy fiber reinforced polymer composites. Zhou et al.[13] established a 3D computational studies of the damage and fracture in the CNT reinforced carbon fiber composites and compared with the experimental results.

Previous works mostly treat the CNT on the carbon fiber as a reinforced component and establish the three phase model: fiber, effective interphase (CNT reinforced matrix) and matrix. HCF pullout test simulation is a complex process. During the CNT pullout from the matrix, the mechanical properties of the effective interphase is uncertain. So in the present work, we combine the single carbon nanotube pullout theory and the CZM in order to account for the effect of CNT on the HCF/matrix interfacial strength. The investigation of the CNT parameters is then extended to quantify the effects of the interfacial shear strength during the fiber pullout test.

2. Model

2.1. Theoretical model for CNT pullout at microscale

For the HCF material, the size of CNT and carbon fiber is at microscale and macroscale, respectively. We utilize a theoretical model to characterize the effect of CNT on the surface of carbon fiber during the pullout test.

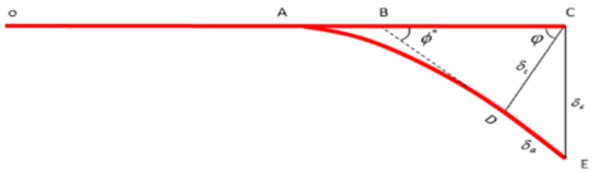

Figure 2. Mechanical model of single CNT pullout from matrix.

The mechanical model of CNT pullout from the matrix as shown in **Figure 2**. For simplification, we focus on the maximum pullout stress σ_p from the carbon fiber at CNT/CF connected surface and the maximum debonding displacement δ_d. which is divided into two parts: the axial displacement δ_a of CNT and the compression displacement δ_c attributed to the compression of matrix σ_c. The compressive stress σ_c is as assumed to be a constant compression distributed on the half surface of CNT. In this paper, we employ the curve coordinate system s along the axial of CNT. s=0 means the end of CNT away from the carbon fiber surface [14]. CNT is regarded as cylinder and the length and radius of CNT are l_f and r_f, respectively. The length of straight segment OA of CNT is z. The rotational angle ϕ is the angle between the initial axial direction CNT and the tangent direction CNT. The compression angle φ is the angle between the initial axial direction CNT and compression displacement direction.

During the HCF pullout process, we have the boundary condition $\sigma(s=l_f)=\sigma_p$ at the connected region between CNT and carbon fiber surface. The axial displacement δ_a in debonding stage contains the elongations of bent segment and straight segment, which can be expressed as:

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$$\delta_a = \frac{1}{E_f}\left(\frac{\mu\sigma_c - 2\tau_i}{2r_f} z^2 + \sigma_c l_f - \frac{\mu\sigma_c l_f^2}{2r_f} \right) \tag{1}$$

where E_f is the elastic modulus of CNT; μ is the friction coefficient at the CNT/matrix surface; τ_i is the shear stress at the CNT/matrix surface.

Then substituting the boundary condition $s(\phi=0)=z$ and $s(\phi=\phi^*)=l_f$ into Eq (1), we can get the following relationship between axial displacement δ_a and pullout stress σ_p in the debonding stage:

$$\delta_a = A_1\sigma_p^2 + A_2\sigma_p \tag{2}$$

where $A_1 = \frac{r_f}{2\mu\sigma_c E_f}\left(1 - e^{-\frac{\pi\mu\phi^*}{2}}\right)$ and $A_2 = \frac{l_f}{2E_f} e^{-\frac{\pi\mu\phi^*}{2}}$.

In order to obtain the relationship between compression displacement δ_c and pullout stress σ_p , we refer to the derivation in Ref.[14]:

$$\delta_c = \sqrt{A_3^2 + \left(A_4 - A_5\right)^2 + 2A_3\left(A_4 - A_5\right)\cos\phi^*}\,\sigma_p = A_6\sigma_p \tag{3}$$

The detail parameters are expressed as follows:

$$\begin{aligned} A_3 &= \frac{\pi r_f}{\sigma_c\left(4 + \pi^2\mu^2\right)\sin\phi^*}\left[2e^{-\frac{\pi\mu\phi^*}{2}} + \left(\pi\mu\sin\phi^* - 2\cos\phi^*\right)\right] \quad A_5 = \frac{r_f}{\mu\sigma_c}\left(1 - e^{\frac{\pi\mu\phi^*}{2}}\right) \\ A_4 &= \frac{\pi r_f}{\sigma_c\left(4 + \pi^2\mu^2\right)\sin\phi^*}\left[2 - e^{-\frac{\pi\mu\phi^*}{2}}\left(\pi\mu\sin\phi^* - 2\cos\phi^*\right)\right] \end{aligned} \tag{4}$$

In this paper, we focus on $\phi^*=\pi/2$ situation, then it can be obtained the following relationship between maximum pull stress σ_p and the debonding displacement δ_d :

$$\sigma_p = \frac{-\left(A_2 + A_6\right) - \sqrt{\left(A_2 + A_6\right)^2 + 4A_1\delta_d}}{2A_1} \tag{5}$$

We can also obtain the traction-separation law for the sliding process as follows:

$$\sigma_p = \left(l_f - \delta_{slip}\right)\left[\frac{r_f}{2\tau_f} + A_5\left(1 - \frac{\mu\sigma_c}{2\tau_f}\right)\right]^{-1} \tag{6}$$

where τ_f is the frictional interface stress during the sliding process; δ_{slip} is the sliding separation.

Then, Combining Eq. (5)with Eq.(6), we obtain the traction-separation law of the CNT pullout process described by following equation:

$$\sigma_p = \left(1 - D\right)\frac{-\left(A_2 + A_6\right) - \sqrt{\left(A_2 + A_6\right)^2 + 4A_1\delta_t}}{2A_1} + \frac{D\left(l_f - \delta_t\right)}{\frac{r_f}{2\tau_f} + A_5\left(1 - \frac{\mu\sigma_c}{2\tau_f}\right)} \quad 0 \le \delta_t \le l_f \tag{7}$$

where δ_t is pullout displacement at any pullout stage. σ_p is the corresponding traction stress. D is a damage state variable.

2.2. Cohesive zone model for CNT reinforced fiber/matrix interface

In this paper, we combine the theory in the above section 2.1 with the bilinear CZM [15] in order to reflect the effect of the CNTs radially grown on the surface of carbon fiber as shown in Eq.(8).

$$\tau_{CF} = \begin{cases} \frac{\tau_{\max}}{\delta_0}\delta_t & 0 \le \delta_t \le \delta_0 \\ \frac{\tau_{\max}}{\delta_f - \delta_0}\left(\delta_f - \delta_t\right) & \delta_0 \le \delta_t \le \delta_f \end{cases} \tag{8}$$

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Two assumptions are made to simplify the problem:(1)The CNTs are densely distributed on the surface of carbon fiber. (2)All the CNTs have identical mechanical properties.Based on these assumptions, the shear traction of new CZM is described as follows:

$$\tau=\left(1-\hat{D}\right)\sum_{i=1}^{N}S_{CNT}^{i}\left(1-D\right)\frac{-\left(A_2+A_6\right)-\sqrt{\left(A_2+A_6\right)^2+4A_1\delta_t}}{2A_1S_{CF}}+\frac{D\left(1-\hat{D}\right)\left(l_f-\delta_t\right)}{\frac{r_f}{2\tau_f}+A_5\left(1-\frac{\mu\sigma_c}{2\tau_f}\right)}+\tau_{CF} \qquad (9)$$

where N is the total number of CNTs distributed on the surface of carbon fiber. S_{CNT} is the area of the single CNT connected to the carbon fiber, S_{CF} is the surface area of the carbon fiber. $\hat{D}$ is the interface damage variable.

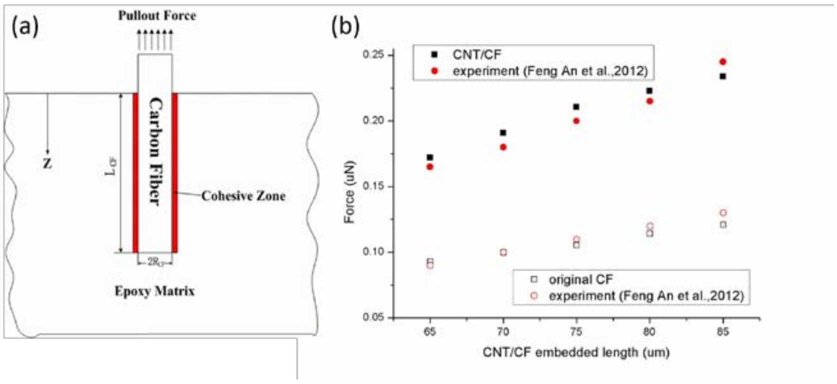

Figure 3. (a)Axisymmetric finite element model for HCF pullout test (In this figure the red zone is the modified cohesive interface).(b) Numerical results of peak force versus a linear function of embedded length.

3. Results and discussion

3.1. Single HCF pullout simulation

In **Figure 3(a) ,** an axisymmetric FE model is set up with the geometrical and loading parameters identical to the test reported. For example, fiber radius R_{CF}=3.5 μm and the embedded length of carbon L_{CF}=75 μm, the width of the model is 100 μm, the interfacial parameters of CNT/matrix[16], parameters of the bilinear CZM [15] and distribution density of CNTs [4] are listed in Table 1. The matrix is defined as the isotropic elastic material, and the carbon fiber is defined as the transversely isotropic elastic material .The detail parameters are listed in Table 2.

Table 1. Interface parameters

CNT radius	CNT length	Young's modulus	Shear strength	Compress stress	Friction	Characteristic displacement	Crack displacement	Interfacial crack initiation stress
r_f (μm)	L_f(μm)	E_f (GPa)	τ_s(MPa)	σ_c (MPa)	μ	δ_0 (μm)	δ_f (μm)	τ_{max}(MPa)
0.03	6.5	496	60.52	60	0.2	21.86	25	68

Table 2. Material properties of carbon fibers and matrix

CF transverse Young's modulus	CF Axial Young's modulus	CF Transverse shear modulus	CF Axial shear modulus	CF Axial poisson's ratio	Matrix Young's modulus	Matrix poisson's ratio
E_1 (GPa)	E_2 (GPa)	G_{13}(GPa)	G_{13}(GPa)	ν_{13}	E_m(GPa)	ν_m
15	230	7	27	0.013	3.4	0.36

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We establish the FE model with the new CZM and calculate maximum pullout force in our model. The original carbon fiber pullout process is also modelled in our work. As shown in **Figure 3(b)**, it is found that our numerical simulation agrees well with the experiment, which validates that the new CZM can successfully describe the interfacial behavior of the HCF during the pullout process.

3.2. Parameters discussion

In this section, we study the effect of some parameters such as the distribution density of CNT and the aspect ratio of CNT on the interfacial mechanical properties of the HCF composites. Under the same volume fraction of CNT, the distribution density varies from 15 tubes/μm^2 to 30 tubes/μm^2 and aspect ratio of CNT varies 150 to 550. **Figure 4** shows the influence of distribution density and aspect ratio on the interfacial shear strength (IFSS) during the pullout process. It is clearly found that IFSS increases approximately linear with the increase of aspect ratio in any case. Meanwhile, this figure demonstrates that IFSS is also ascend as the distribution density increases.

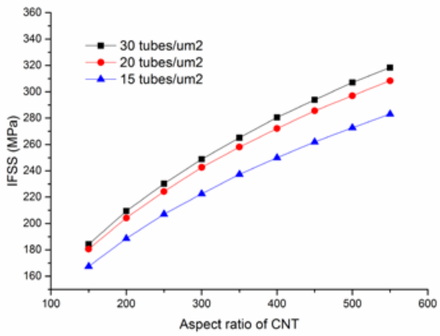

Figure 4. IFSS of fiber pullout vs aspect of ratio of CNT curves for different parameters about distribution density of CNT under the condition of the same volume fraction of CNT.

3. Conclusions

In this paper, a new CZM of composites is proposed to simulate the HCF pullout process. We combine the CNT pullout theory and CZM using the user-defined element in ABAQUS software. The effect of CNT at microscale is added into the cohesive elements at macroscale during the HCF pullout process.
An axisymmetric finite element model with the interface element is proposed to simulate the single fiber pullout test with the purpose of the verification. Simulation results show that the numerical model can better fit the experimental results, which indicates the validity of the new CZM. The new CZM can demonstrate that CNTs improve the stiffness of the interface and reinforce the mechanical property of the interface. The result shows that interfacial shear strength increases with the enhancement of aspect ratio and distribution density under the same volume fraction of CNT,which provide theoretical help for the experimental preparation of HCF materials.

Acknowledgments

The authors thank the support from the National Natural Science Foundation of China (11472025 and 11272030).

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