MICROMECHANICAL MODELING OF DOUBLE-WALLED CARBON NANOTUBE PULLOUT FROM A MATRIX

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Abstract
In the paper, a micromechanical model of double-walled carbon nanotube (DWCNT) pullout from a matrix is presented with the interfacial residual stress and van der Waals (vdW) force taken into account. The interfacial residual stress induced by thermal expansion coefficient (TEC) mismatch is introduced via thermo-elastic constitutive relations. The effects of vdW interaction between two layers of DWCNT on the interfacial stress of DWCNT and matrix are analyzed. Then the analytical expressions of interfacial shear stress and the axial stresses of DWCNT and matrix are derived, respectively. Furthermore, the influences of temperature change, interfacial friction coefficient, DWCNT aspect ratio, DWCNT volume fraction and the relative modulus between DWCNT and matrix are illustrated and discussed.

1 Introduction
Carbon nanotubes (CNTs) are regarded as the promising reinforcing phase in the advanced composites, due to their superior physical and mechanical properties, low density, superior toughness and extreme high surface-to-volume ratio. However, the studies [1-4] show that the mechanical properties of the CNTs-reinforced composite materials do not get large improvement. Carbon nanotubes do not bond well to the matrix materials [4-5], and the sliding of CNTs will occur when subjected to loading. The composites usually damage on the interface of CNTs/matrix. Therefore, the interfacial stress transfer efficiency has significantly influence on the mechanical properties of composites.

The interfacial mechanical behavior between the CNTs and matrix has attracted much attention of researchers. Lots of experimental studies [1-6] have been done to investigate the interfacial stress transfer between CNTs and matrix. Although there are some theoretical analyses [7-12], these models are similar to those of fibers and matrix. Micromechanical effects were not taken into account in the models. In fact, due to large surface-to-volume ratio of the CNTs, the interfacial micromechanical effects, such as van der Waals (vdW) force, etc., will play important roles. Some studies have discussed the influence of vdW force in the process of load transfer by molecular dynamics simulations [13-15]. A theoretical model was presented by Ref.[12] taking the effects of vdW interaction between the graphene layers of MWCNT into account, but the effects of residual stress were not considered in the research. In fact, the residual stress can not be neglected for CNTs reinforced composites since the TEC of CNTs is usually far smaller than the matrix [6]. Until now, there is not a model which takes the residual stress and vdW force into consideration simultaneously.

2 Micromechanical modeling of DWCNT pullout
A three-dimensional axisymmetric two-cylinder model is applied to investigate the pullout of a DWCNT from a matrix. The geometrical dimensions in the model are specified in the Fig.1. A pullout stress σ_p is applied to one end of the DWCNT where $x=L$. There exists a compression pressure q on the interface of DWCNT and matrix, which consists of pressure induced by vdW effects [12, 16], thermal

residual stress and pressure caused by Poisson's effects when the matrix is stretched. The pressure q can be derived via thermo-elastic constitutive relation and the displacement boundary conditions [16] on the interface as,

$$q = \lambda_1 \sigma_{tx}(x) + \lambda_2 \bar{\sigma}_{mx}(x) + \sigma_{RT}\,, \qquad (1)$$

where $\sigma_{tx}(x)$ is the axial stress of the DWCNT and $\bar{\sigma}_{mx}(x)$ the average axial stress of the matrix, λ_1 and λ_2 are coefficients which depended on the physical properties and geometry dimensions of DWCNT and matrix, and σ_{RT} is the residual normal stress arising from the TEC mismatch between CNTs and matrix. The coefficients λ_1 and λ_2 and residual normal stress σ_{RT} can be derived as follows,

$$\lambda_1 = \frac{t}{\xi\Omega} \cdot \left[\frac{v_t}{a_1^2}\left(\frac{E_t t}{a_2^2} + c_0 \right) + \frac{c_0 v_t}{a_1 a_2} \right], \qquad (2)$$

$$\lambda_2 = \frac{v_m}{\Omega E_m}\,, \qquad (3)$$

$$\sigma_{RT} = \left(\frac{\alpha_m}{\Omega} - \frac{\lambda_1 E_t \alpha_t}{v_t} \right) \cdot \Delta T\,, \qquad (4)$$

$$\Omega = \frac{1}{E_m}\left(\frac{b^2 + a_1^2}{b^2 - a_1^2} + v_m \right) + \frac{1}{\xi}\left(\frac{E_t t}{a_1 a_2^2} + \frac{c_0}{a_1} \right), \qquad (5)$$

$$\xi = \left(\frac{E_t t}{a_1^2} + c_0 \right)\left(\frac{E_t t}{a_2^2} + c_0 \right) - c_0^2\,, \qquad (6)$$

where E, v and α are elastic modulus, Poisson's ratio and thermal expansion coefficient, and subscripts 't' and 'm' denote carbon nanotube and matrix, respectively. The parameters b, a_1 and a_2 are radius (as shown in the Fig.1), and t is the thickness of CNTs wall, which is about 0.34 nm. ΔT is the temperature change, which is equal to the test temperature minus the stress-free temperature. The parameter c_0 can be calculated [16, 17] via the equation $c_0 = \frac{200\,\mathrm{erg/cm^2}}{0.16 d^2}$, which is dependent on the vdW interaction between two layers of the DWCNT.

It is assumed that the interfacial shear stress between the DWCNT and the matrix follows the Coulomb friction law, when the debonding of DWCNT occurs. Then the interfacial shear stress can be obtained by

$$\tau_t(x) = \mu \cdot q\,, \qquad (7)$$

where μ is the friction coefficient.

According to the equilibrium of the interfacial shear stress and the DWCNT axial stress, we have

$$\frac{d\sigma_{tx}(x)}{dx} = \frac{2\pi a_1}{A_{eff}} \cdot \tau_t(x)\,, \qquad (8)$$

where A_{eff} refers to the effective cross-sectional area of the DWCNT, which can be calculated by $A_{eff} = 2\pi t(a_1 + a_2)$.

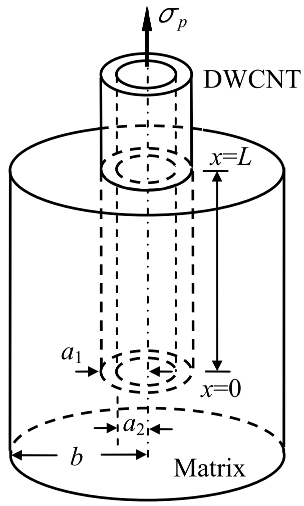


Fig.1. Schematic illustration of the DWCNT/matrix pull-out model.

Furthermore, the static equilibrium equation of the composites can be written as

$$A_{eff}\sigma_p = \pi\left(b^2 - a_1^2\right)\bar{\sigma}_{mx}(x) + A_{eff}\sigma_{tx}(x)\,, \qquad (9)$$

From the equations (7)-(9), a differential equation about the DWCNT axial stress can be obtained,

$$\frac{d\sigma_{tx}(x)}{dx} + h_1 \sigma_{tx}(x) + h_2 = 0\,, \qquad (10)$$

where the coefficients h_1 and h_2 are, respectively,

$$h_1 = -\frac{2\pi\mu a_1}{A_{eff}}\left[\lambda_1 - \frac{A_{eff}}{\pi\left(b^2 - a_1^2\right)} \cdot \lambda_2 \right], \qquad (11)$$

$$h_2 = -\frac{2\pi\mu a_1}{A_{eff}}\left[\sigma_{RT} + \frac{A_{eff} \cdot \sigma_p}{\pi\left(b^2 - a_1^2\right)} \cdot \lambda_2 \right]. \qquad (12)$$

The solution of the differential equation (10) has following form,

$$\sigma_{tx}(x) = h_3 e^{-h_1 x} - h_2/h_1\,, \qquad (13)$$

where h_3 is constant, which can be derived via the stress boundary conditions $\sigma_{tx}(L) = \sigma_p$. Substitute the stress boundary conditions into the equation (13), we have

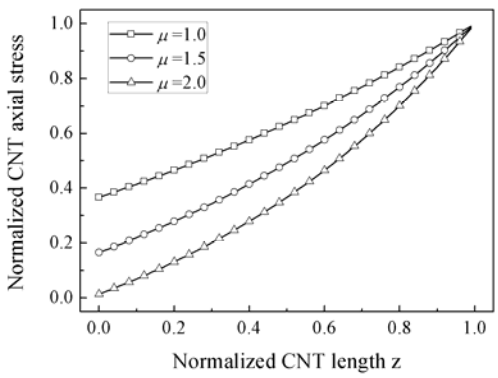
$$h_3 = \left(\sigma_p + h_2/h_1\right)e^{h_1 L}. \quad (14)$$

What is more, substitute equation (13) into the equations (8) and (9), and the interfacial shear stress and matrix axial stress can be derived, respectively,

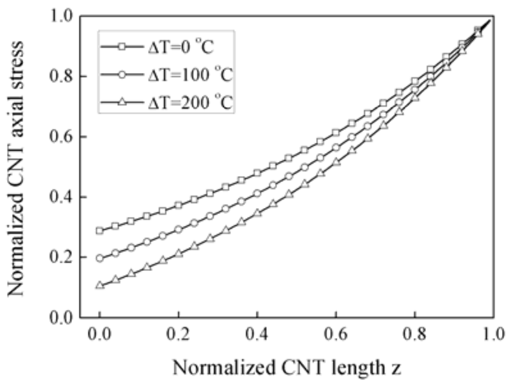
$$\tau_t\left(x\right) = -\frac{A_{eff}h_1h_3}{2\pi a_1}e^{-h_1 x}, \quad (15)$$

$$\bar{\sigma}_{mx}\left(x\right) = \frac{A_{eff}}{\pi\left(b^2 - a_1^2\right)}\cdot\left(\sigma_p - h_3e^{-h_1x} + \frac{h_2}{h_1}\right). \quad (16)$$

3 Results and discussion



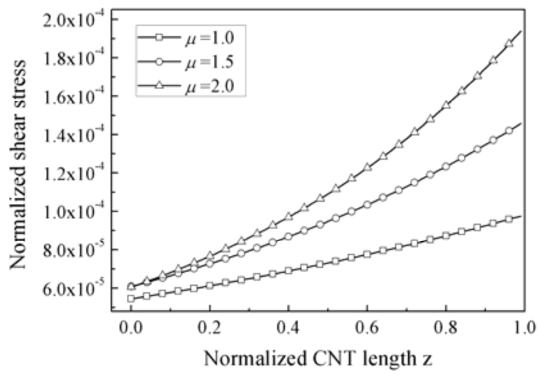
(a)



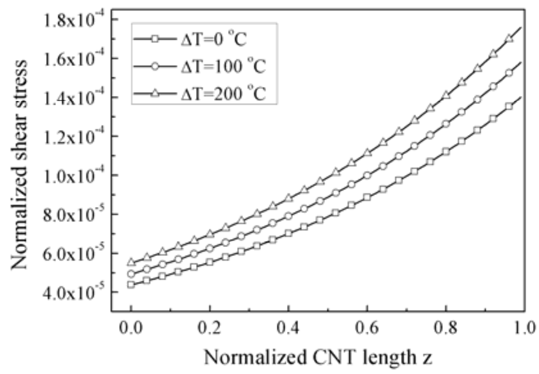
(b)

Fig.2 The distributions of normalized CNT axial stress, $\hat{\sigma}_t = \sigma_{tx}(x)/\sigma_p$, along normalized CNT length, $z = x/L$, (a) for different friction coefficient; (b) for different temperature change.

The interfacial shear stress and DWCNT axial stress are critical factors which control the efficiency of stress transfer and some important mechanical properties of composite such as effective Young's modulus, tensile strength and fracture toughness. Hence, numerical calculations are given in the section for a hypothetical DWCNT composite system to illustrate the distributions of the interfacial shear stress and DWCNT axial stress. The values of parameters applied in the numerical calculation are, respectively, t=0.34 nm, d=0.142 nm, b=100a_1, L=2800a_1, E_t=1.1TPa, E_m=3.5GPa, μ_t=0.34, μ_t=0.48, $\alpha_m = 45\times10^{-6}\ °C^{-1}$, $\alpha_t = -1.5\times10^{-6}\ °C^{-1}$ [18]).



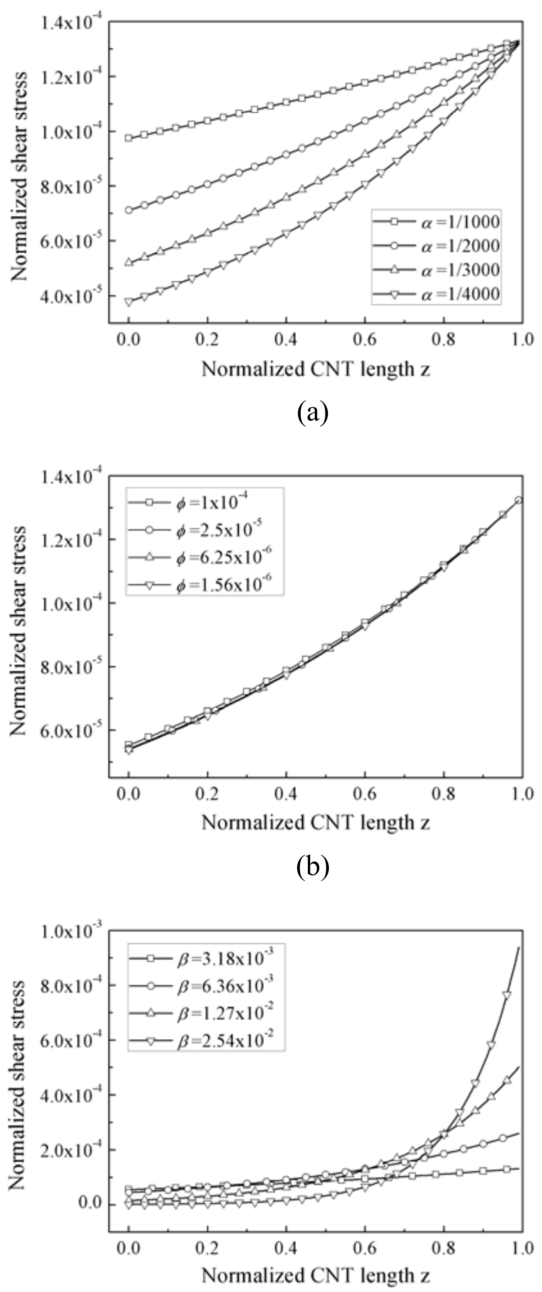
(a)



(b)

Fig.3 The distributions of normalized interfacial shear stress, $\hat{\tau}_t = \tau_t(x)/\sigma_p$, along normalized CNT length, $z = x/L$, (a) for different friction coefficient; (b) for different temperature change.

Fig.2 shows the distributions of normalized DWCNT axial stress along normalized DWCNT length for different friction coefficient and temperature change. It can be seen form Fig.2 that the average DWCNT axial stress decreases when the magnitude of friction coefficient and temperature change increases. The reasons may attribute to that more pullout force is shared by the matrix. It can be concluded that the increase of friction coefficient and thermal residual stress improves the efficiency of stress transfer.



(a)

(b)

(c)

Fig.4 The distributions of normalized interfacial shear stress, $\hat{\tau}_t = \tau_t(x)/\sigma_p$, along normalized CNT length, $z = x/L$, (a) for different CNT aspect ratio, $\alpha=a_1/L$; (b) for different CNT volume fraction, $\phi = a_1^2/b^2$; (c) for different relative modulus between the CNT and matrix, $\beta=E_m/E_t$.

Fig.3 shows the distributions of normalized interfacial shear stress along normalized DWCNT length for different friction coefficient and temperature change. It can be seen form Fig.3 that the maximum interfacial shear stress occurs at the pullout end, z=1, and the interfacial shear stress between DWCNT and matrix increases as the magnitude of friction coefficient and temperature change increases.

In addition, the CNT aspect ratio α, relative modulus between the CNT and matrix β and CNT volume fraction ϕ also have influence on the interfacial stress transfer (as shown in Fig.4). It can be seen from Fig.4a that the normalized shear stress increases as the CNT aspect ratio increases. Simultaneously, the distributions of interfacial shear stress tend to be linear as the CNT aspect ratio increases. From Fig.4b, it can be concluded that the influence of CNT volume fraction on the interfacial shear stress can be neglected. The relative modulus between the CNT and matrix affects the maximum interfacial shear stress. It can be seen from Fig.4c that the maximum interfacial shear stress increases with the enhancement of matrix Young's modulus.

4 Conclusion

A micromechanical model of DWCNT pullout from a matrix is presented with the thermal residual stress and vdW effects taken into account simultaneously. The vdW pressure between two layers of DWCNT is introduced in the model, and the Poisson's effects and thermal effects of DWCNT and matrix are also taken into account by the thermo-elastic constitutive equation. According to Coulomb friction law, the equilibrium of the interfacial shear stress and the DWCNT axial stress and the continuous condition of displacement and stress on the interface, the interfacial shear stress, DWCNT axial stress and matrix axial stress are derived, respectively. Furthermore, the influence of following factors is illustrated and discussed by numerical calculations: temperature change, interfacial friction coefficient, CNT aspect ratio α, relative modulus between the CNT and matrix β and CNT volume fraction ϕ. The influence of CNT volume fraction can be neglected, but other factors have important influence on the distributions of interfacial stress.

Acknowledgements

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