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Multi-scale modeling of carbon nanotube reinforced composites with a fiber break

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ABSTRACT

Present paper deals with the study of stress distribution in the vicinity of a broken carbon nanotube (CNT) in CNT-based fiber reinforced composites. Three dimensional finite elements analysis (FEA) using multi-scale modeling has been done considering a square representative volume element (RVE) and the effect of a broken CNT on the adjacent CNTs and on the matrix has been studied for CNT/Epoxy and CNT/Titanium composites. The distributions of stresses in the broken CNT, at the interface, and in the adjacent CNTs have been analyzed for different volume fractions. It is observed that the ineffective length of the broken CNT is dependent on the volume fraction as well as on the type of matrix materials. The magnitude of the interfacial shear stress as well as the stress concentration in the vicinity of the broken CNT is also influenced by the fiber volume fraction and the type of matrix materials.

1. Introduction

Carbon nanotubes not only exhibit exceptionally high stiffness, strength and resilience but also possess superior electrical, thermal and mechanical properties. These nanotubes are also chemically inert and are able to sustain a high strain without breakage. These properties of CNTs are believed to be ideal for using them as reinforcements in high performance structural composites. Therefore, among many potential applications of nanotechnology, nanocomposites have been one of the latest research areas in the recent years and hence a large number of works has already been reported in the direction of modeling and characterization of CNT-based composites. Due to their extremely small sizes, analytical models are difficult to be established, fabrication process and tests are extremely difficult and expensive to conduct. On the other hand, modeling and simulation can be advantageously used to analyze such nanocomposites. In spite of all the advantages, sometimes the CNT-based composites may have one or more CNTs broken. This may be due to manufacturing defect or in-service damage. Therefore, the investigation of the stress redistribution as a result of the presence of a broken CNT is one of the important issues which need to be addresses from the view point of failure of such CNT reinforced composites.

Carbon nanotubes are fullerene-related structured discovered by Iijima [1]. Earlier works [2,3] determined the elastic and mechanical properties of CNTs and reported that the Young's modulus and Poisson's ratio of CNTs were in the order of 1 TPa and 0.28, respectively. Thostenson et al. [4] and Lau and Hui [5] presented a comprehensive review on manufacturing processes, mechanical and electrical properties and applications of CNT-based composites. Odegard et al. [6] proposed a method for developing structure–property relationships of nano-structural materials. Montazeri et al. [7] investigated the mechanical properties of multi-walled CNT (MWCNT)/Epoxy composites and concluded that acid-treated MWCNT was more efficient as reinforcement in Epoxy matrix than untreated MWCNT. Lau and Hui [8] reported that the use of MWCNTs as intrinsic reinforcements for composite structures might not allow the maximum strength to be achieved due to non-uniform axial deformation inside the MWNTs and hence the use of single-walled carbon nanotubes (SWCNTs) might be more beneficial for advanced composites structures. Effective mechanical properties of CNT-based composites are evaluated using a 3-D nanoscale RVE based on the 3-D elasticity theory and solved by the finite element method (FEM) by Chen and Liu [9]. Lusti and Gusev [10] performed FE analysis for calculation of Young's modulus and coefficients of thermal expansion (CTE) of CNT/Epoxy composites for different fiber orientation of CNTs in matrix, and concluded that CNTs could be more efficient as compared to conventional glass or carbon fibers.

Load transfer depends on the interfacial shear stress between the fiber and matrix and the performance of a composite materials system is critically controlled by the interfacial characteristics of the reinforcement and the matrix material. Wagner et al. [11] reported the shear stress transfer ability of MWCNT/polymer interface to be more than that of current advanced composites and was of the order of 500 MPa. Cooper et al. [12] found from pullout experiments that the interfacial shear stress between a MWCNT and Epoxy ranged from 35 to 375 MPa. Barber et al. [13] performed pullout experiment using atomic force microscopy and found that

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the separation stress is remarkably high, indicating the efficacy of CNTs as reinforcement in polymer. Qian and Dickey [14] conducted experiments and concluded that with only 1% (by weight) addition of CNTs in polystyrene (PS), elastic modulus and breaking stress were observed to increase by 36–42% and 25%, respectively. Meguid and Sun [15] experimentally determined the influences of debonding and shear characteristics at the interfaces of nanocomposites at different volume fractions. Haque and Ramasetty [16] developed an analytical model to study the stress transfer in SWCNT reinforced polymer matrix composites. Li and Saigal [17] developed a micromechanical model for assessing the interfacial shear stress transfer in CNT-reinforced polymer composites. Gao and Li [18] developed a shear-lag model for predicting the interfacial stress transfer in CNT-reinforced polymer composites using a multi-scale approach. Xiao and Zhang [19] investigated the effects of nanotube length and diameter on the distributions of tensile stress and interfacial shear stress of SWCNT in Epoxy matrix. Multiscale modeling of carbon nanotube reinforced polymer composites is required to simulate and assess the true response of CNT-based composites. Li and Chou [20] analyzed the stress distribution in CNT/polymer composites subjected to tension by combining the atomic molecular structural mechanics approach and the continuum FEM. Tserpes et al. [21] proposed a multi-scale RVE for modeling of tensile behavior of CNT-reinforced composites.

There are many literatures available in the broad area of CNT-based composites and most of these studies were related to the elastic and mechanical properties of nanocomposites. There are some literatures also available describing the manufacturing processes like resin transfer molding, sonication techniques, powder metallurgy and spark plasma sintering processes commonly used for manufacturing CNT/Epoxy as well as CNT/Titanium composites [7,22–25]. All these literatures reported the load carrying capacity of CNTs to be significant and CNT-based composites had a potential to provide extremely strong and ultra lightweight new materials. In spite of all these advantages, one or more CNTs may break due to different reasons and it is possible that a CNT based composite is having broken CNTs in it. Therefore it is important to understand the influence of such broken CNTs in the nanocomposites in terms of stress redistribution and possibilities of failure. However, there is no work available on the study of stress distribution in the vicinity of a broken CNT in the CNT-based composites. Nedele and Wisnom [26] analyzed the stress concentration at a single fiber break for a conventional fiber reinforced composites using FEM. Therefore the present paper aims at studying the effect of a broken CNT in the composite in the form of normal and shear stress redistribution surrounding the broken CNT in a CNT-based composite and to study the effect of different important parameters on the failure of such composites.

2. Atomic structure of CNTs

CNTs are three types viz. zigzag, armchair, and chiral. Fig. 1 shows the different types of CNTs formed from a hexagonal graphene sheet. If the rectangle (*ABCD*) is cut from the graphene sheet and rolled up in such a way that the tip (*B*) of the chiral vector ($\mathbf{C}_h$) touches its tail (*A*), chiral CNT is produced. The atomic structure of CNTs can be described by the tube chiral vector and chiral angle (θ). The chiral angle determines the amount of twist in the tube. If $\theta = 0°$ and $30°$ it will form zigzag and armchair CNTs, respectively and for $0° < \theta < 30°$, it will form chiral CNT. The chiral vector also known as the roll-up vector and it can be described by the following equation

$$\mathbf{C}_h = n\mathbf{a}_1 + m\mathbf{a}_2 \tag{1}$$

where the integers (n, m) are the number of steps along the zigzag carbon bonds and $\mathbf{a}_1$ and $\mathbf{a}_2$ are unit vectors as shown in Fig. 1.

The circumference of the CNTs also determine by the following equation

$$L = |\mathbf{C}_h| = a\sqrt{n^2 + m^2 + nm} \tag{2}$$

where a is the length of unit vector.

3. Multi-scale modeling of CNT-reinforced composites

A square RVE having nine uniformly spaced CNTs in the matrix has been considered for the analysis. Most of the earlier literatures have considered the linear behavior of CNTs in CNT-based composites. But in reality for larger deformation, CNTs behave nonlinearly and the nonlinear behavior of CNT needs to be considered for the analysis.

The stress–strain curves of the armchair and zigzag CNTs were found experimentally by Tserpes et al. [21] and by fitting the data of the curves using third order polynomials, they obtained the following relations between the stress and strain

$$\sigma_n = 2909.8\varepsilon_n^3 - 4995.6\varepsilon_n^2 + 1364.9\varepsilon_n \quad \text{(for zigzag CNT)} \tag{3}$$

$$\sigma_n = 5958.5\varepsilon_n^3 - 4769.4\varepsilon_n^2 + 1334.7\varepsilon_n \text{(for armchair CNT)} \tag{4}$$

Eq. (3) has been used in the present analysis considering zigzag CNT.

In the present work, two different types of matrix materials viz. Epoxy and Titanium have been chosen to study the effect of matrix materials on the stress distribution around the broken CNT in the CNT-based composites. Properties of matrix materials [26,27] are as follows

$$\text{Epoxy}: \quad E_m = 3.89\ \text{GPa}, \quad \nu_m = 0.37$$

$$\text{Titanium}: \quad E_m = 116\ \text{GPa}, \quad \nu_m = 0.32$$

For zigzag SWCNT, Eq. (3) has been used along with $\nu_{nt} = 0.28$.

4. Modeling of CNT-reinforced composites with a broken CNT

4.1. Three dimensional FE model

In order to study the effect of a broken CNT on the adjacent CNTs as well as in the interface and matrix, a square RVE with 9-CNTs (refer Fig. 2) have been considered. The diameter of CNT has been taken as 1.88 nm (which is equal to the diameter of zigzag (24, 0) CNTs) and the thickness (t) of CNT layer is considered 0.34 nm. The length of the CNT has been taken as 100 nm.

The broken fiber is considered to be placed at the center of the RVE which is surrounded by the matrix materials. Since the RVE is modeled with 9-CNTs, the broken CNT is surrounded by eight neighboring intact CNTs. SOLID45 elements embodied in ANSYS have been used for modeling the RVE. A refined mesh has been used near the broken CNT. At $z = 0$ the length of the element is smallest and it is gradually increased along axial direction of the composites. The front view and pictorial view of the 3-D FE model of the square RVE are shown in Fig. 2a and b, respectively for a constant volume fraction 3.056% of CNT.

4.2. Boundary conditions

A 3-D FE model for a RVE with 9-CNTs is shown in Fig. 2, where the x–y plane is the transverse plane and the z-axis is the axial direction. All the nodes at $z = 0$ are fully restrained except the nodes belonging to the broken fiber. The axial mechanical loading of the nanocomposites is applied by a uniform displacement in the axial direction at the far end of the model i.e. at nodes at $z = L_a$, where L_a is the axial length of the model. The displacement increment was chosen equal to 1% of the length of the model. The total