MICRO- AND NANO-MECHANICS OF CARBON NANOTUBES COMPOSITES

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Summary In the present paper, the constitutive relation and failure behaviorsof carbon nanotube-reinforced composites are studied using methods of micromechanics and nanomechanics. First, we examined the factors that influence the overall mechanical property of carbon nanotube composites, including the weak bonding between carbon nanotubes and matrix, the curviness and agglomeration of carbon nanotubes. Second, we established a hybrid continuum/micromechanics/atomistic method to investigate the defect nucleation in a carbon nanotube embedded in a polymer matrix.

INTRODUCTION

Both experimental and theoretical studies have shown that carbon nanotubes (CNTs) have extraordinary mechanical and electrical properties [1, 2]. Such superior properties make CNTs a very promising candidate as the ideal reinforcing fibers for advanced composites with high strength and low density. Though some encouraging results have been reported, there are many other experiments that demonstrate only modest improvement in the strength and stiffness after CNTs are incorporated into polymers. Why there are no consistent improvements in mechanical properties of CNT-reinforced composites? This is investigated in this paper and it is shown that the unsatisfactory improvement in the mechanical properties of CNT-reinforced composites could be attributed to the weak bonding and interaction between CNTs and polymer matrices, as well as the waviness and agglomeration effects of CNTs. In addition, we presented a combined continuum/micromechanics/atomistic method to investigate the defect nucleation and fracture behaviours of CNTs in polymers.

STIFFENING MECHANISMS OF CARBON NANOTUBES

Waviness effect

Because CNTs have very low bending stiffness due to the small tube diameter (~ 1 nm), most CNTs in composites exist in a curved state. However, there is yet no theoretical model to estimate the stiffening effect of curved CNTs. We presented here a micromechanics model to examine the waviness effect of curved CNTs on the elastic properties of CNT-reinforced composites. A unit cell is chosen containing a curved CNT, which is modeled as a helical spring and its waviness is governed by the spiral angle. The RVE is divided into slices of infinitesimal thickness to estimate the stress and strain fields in the unit cell. The Mori-Tanaka method is employed to estimate the stiffening effect of curved CNTs. Some examples are given to show the dependence of the effective elastic modulus of composites as a function of the elastic constants and the volume fraction of CNTs having different wavinesses and orientation distributions. It is observed that the modulus of carbon nanotube composites decreases rapidly as the waviness increases.

Agglomeration effect

Due to their low bending stiffness and high aspect ratio, CNTs are very easy to agglomerate in the polymer matrix. We develop a micromechanics model to study the influence of the agglomeration of CNTs on the effective elastic moduli of CNT-reinforced composites. The spatial distribution of CNTs in the matrix is assumed to be non-uniform such that some local regions have a higher concentration of CNTs than the average volume fraction in the material. These regions with concentrated CNTs are assumed to have spherical shapes, and are considered as "inclusions" with different elastic properties from the surrounding material. Thus, we consider the CNT-reinforced composite as a system consisting of inclusions of sphere shape embedded in a hybrid matrix. Both the matrix and the inclusions contain CNTs. This model have two parameters describing the agglomeration of CNTs. We estimate the effective elastic stiffness of the composite containing either straight or curved CNTs by using the above micromechanics. The changing curves of the effective tensile moduli with the agglomeration parameters are given. It is clearly shown that the agglomeration of CNTs exerts a significant weakening effect to CNT-reinforced composites. In addition, the anisotropic property of CNTs affects to a considerable extent the overall effective elastic moduli, especially the Young's modulus at uniform distribution.

Interface effect

Interfaces often play a significant role in mechanical and physical properties of nanostructured materials. For CNT-reinforced composites, the high surface area of CNTs creates a large interfacial region, which has properties different from the bulk matrix. We used a three-phase unit cell method to calculate the impact of interface adhesion on the effective elastic moduli of composites. This micromechanics method can easily derive the effective moduli of composites with good accuracy, even for a high volume fraction of inclusions. It is assumed that each CNT is assumed to have very high length-to-radius ratios and considered as fibers of infinite length. For polystyrene composites reinforced with aligned CNTs, the tensile elastic moduli are given as a function of the parameters of interfaces. For a weak interface, the effective elastic moduli are insensitive the interface thickness. Therefore, the unsatisfying improvement of the stiffness of CNT-reinforced composites observed experimentally cannot be explained by the interface effect. These results can be easily understood because the axial elastic modulus of CNTs is much higher than those of the polymer matrix and the interface phase, and so the stiffening effect of CNTs is predominated by the elastic constants, geometric parameters, spatial distribution and microstructures of CNTs in composites.

DEFECT NUCLEATION AND FRACTURE OF NANOTUBES IN COMPOSITES

Hybrid continuum/atomistic method

To investigate the deformation and fracture behaviors of carbon nanotubes, we conducted a hybrid continuum/atomistic study [3, 4] based on the Tersoff-Brenner potential and the Cauchy-Born Rule. Atoms far away from the defect are represented by an atomistic-based continuum theory, which has been shown to agree well with molecular dynamics simulations studies without any parameter fitting. For atoms near the defect, we use molecular mechanics coupled with the atomistic-based continuum theory to determine the atom positions. This hybrid continuum/atomistic study significantly reduces the computation.

Defect nucleation and evolution in carbon nanotubes

The above hybrid continuum/atomistic method is employed to consider the problem of defect nucleation and evolution of CNTs under tension. The tensile stress-strain curves of CNTs are first simulated, without any parameter fitting, as a function of the chiral angle and diameter, and the results agree well with the experimental curves [5]. As the tensile strain reaches a critical value, the so-called Stone-Wales transformation (i.e., 90^{o} rotation of a C-C bond, resulting in a low energy 5-7-7-5 ring pair) occurs. The critical strain of occurrence of a Stone-Wales depends strongly on the chiral angle, and ranges from 8.2% for armchair CNTs and 15.3% for zigzag CNTs. The Stone-Wales defect will become unstable when a second critical load is reached. The fracture paths and instability modes after defect nucleation are dependent also upon the chiral angle.

Fracture of carbon nanotubes embedded in a polymer matrix

To simulate the fracture process of carbon nanotubes interacting with the surrounding matrix, which is of great interest in field of nanomechanics and nanomaterials, we adopted a combined continuum/micromechanics/atomistic method, as an extension of the above analysis of CNTs without interaction with matrix. The far-field stress in the unit cell around a CNT is determined by the Mori-Tanaka method of micromechanics. Our calculations show that the interaction between CNTs and matrix lowers the critical strain of fracture of CNTs, in comparison with that without interaction effect.

CONCLUSIONS

In the present paper, the stiffening and strengthening physical mechanisms of CNTs in polymer matrix are investigated theoretically by using micromechanics and nanomechanics methods. The effect of waviness, agglomeration and interfaces of CNTs are examined. It is established that the waviness and agglomeration may significantly reduce the stiffening effect of CNTs. A combined continuum/micromechanics/atomistic method is developed to simulation the fracture process of CNTs in a polymer. We have given the critical tensile strains of defect nucleation and final fracture, which show a strong dependence on the chiral angle The present study not only provides the important relationship between the effective properties (both elastic modulus and strength) and the microstructure parameters of CNT-reinforced composites, but also may be useful for improving and tailoring their mechanical properties.

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