Micromechanics and multiscale mechanics of carbon nanotubes-reinforced composites

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Abstract

Owing to their superior mechanical and physical properties, carbon nanotubes (CNTs) seem to hold a great promise as an ideal reinforcing material for composites of high-strength and low-density. In the present paper, the stiffening and strengthening physical mechanisms of CNTs in polymer matrix are investigated theoretically by using micromechanics and multiscale mechanics methods. First, the stiffening effect of CNTs in composites is quantitatively examined by micromechanics methods. Second, a hybrid atomistic/continuum mechanics method is established in the present paper to study the deformation and fracture behaviors of CNTs in composites due to the enormous difference in the scales and mechanisms involved in this issue. A unit cell containing a CNT embedded in a matrix is divided in three regions, which are simulated by the atomic-potential method, the quasi-continuum method based on the modified Cauchy-Born rule, and the classical continuum mechanics, respectively. This method can not only predict the formation of Stone-Wales defects, but also simulate the subsequent deformation and fracture process of CNTs embedded in composites. The present study elucidates some key factors (e.g., waviness, agglomeration, residual stress, and interphase) that influence the mechanical properties of CNT-reinforced composites, and therefore may be useful for improving and tailoring their mechanical properties.

Keywords: Carbon nanotube; Composite; Constitutive relation; Fracture; Stone-Wales transformation; Multiscale mechanics method; Micromechanics.

1. Introduction

Since their discovery in 1991 [1], carbon nanotubes (CNTs) have attracted tremendous research interests due to their extraordinary mechanical, physical and chemical properties [2–5]. Much attention has been paid in the past decade to reveal the physical, chemical and other properties of CNTs and to explore their various potential applications in, e.g., novel nano-materials, devices and systems, and ultra-strong composite materials.

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Both theoretical analysis [6–14] and experimental measurements [15–20] evidence that both single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) have Young’s moduli about 1 TPa under uniaxial tension. The Young’s modulus of CNT is a statistically averaged parameter of bonds and defects, and therefore, the results of theoretical calculations and experimental measurements of Young’s modulus generally have a reasonable agreement. However, the tensile strength and breaking strain are sensitive to the local deformation, types and orientations of defects, constraint conditions and some other factors. So the results of theoretical and experimental studies on CNTs strength and fracture often show a pronounced dispersion and inconsistency. The deformation and fracture of CNTs is studied by molecular dynamics simulation in [21]. They found that Stone-Wales transformation is a typical mechanism for fracture nucleation of CNTs and the fracture strains are in the range of 30–55%, depending on temperature. A hybrid atomistic/continuum model was developed to study the mechanical properties of CNTs and predicted an axial breaking strain of about 52%, which corresponds to the onset of deformation bifurcation [22, 23]. Other atomistic studies also predicted that the tensile fracture strains of CNTs could reach up to 30% [24–26]. However, experimental measurements [19, 20, 27, 28] shown that the fracture strains of CNTs are usually less than 13%. Someone [29, 30] conducted atomistic studies on failure of CNTs, and found that the discrepancies between the aforementioned atomistic and experimental studies can be attributed to the non-physical cutoff function in Brenner’s interatomic potential [31] for carbon. Using a modified Morse potential, they predicted the failure strains of CNTs in the ranges of 10–16% and 16–24%, respectively.

In spite of the big dispersion between experimental results and theoretical predictions, it is well accepted that the mechanical properties of CNTs are much better than all the commercial fibers. Such superior properties make CNTs seems to be a very promising candidate as ideal reinforcing fibers for producing advanced composites with high strength and low density, which are of paramount interest in astronautical, aeronautical and other industries. Composites of CNTs dispersed in metallic or polymeric matrices have attracted a considerable attention in recent years [32, 33]. Different kinds of CNT-reinforced composites have been synthesized with enhanced properties. For example, a MWCNT reinforced polystyrene with good dispersion and CNT-matrix adhesion was reported in [34]. Using only 0.5% CNT reinforcement, the elastic modulus and tensile strength were improved about 40% and 25% over those of the matrix, respectively. It was found in [35] that by adding SWCNTs in isotropic petroleum pitch matrices, the tensile strength, elastic modulus, and electrical conductivity of the composite with 5 wt% content of purified SWCNTs were enhanced by about 90%, 150%, and 340%, respectively. It was reported in [36] that the incorporation of 1 wt% MWCNTs reinforcement produced a remarkable increase in the tensile strength and elastic modulus for non-drawn UHMWPE composite films of 49.7% and 38% and, more interestingly, enhanced significantly both the ductility and the strain energy absorption before fracture. However, a big difference still exists between these practical improvements and the expectations predicted from theoretical analysis, and many other studies demonstrated only modest improvement in the strength and stiffness after