Hierarchical Failure Analysis and Optimal Toughness Design of Carbon Nanotube-Reinforced Composites

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Abstract

Hierarchical analysis of the fracture toughness enhancement of carbon nanotube (CNT)-reinforced composites is herein carried out on the basis of atomistic simulation, shear-lag theory and facture mechanics. It is found that neither longer reinforced CNTs nor stronger CNT/matrix interfaces can definitely lead to the better fracture toughness of these composites. In contrast, the optimal interfacial chemical bond density and the optimal CNT length are those making the failure mode just in the transition from CNT pull-out to CNT break. To verify our theory, an atomic/continuum finite element method (FEM) is applied to investigate the fracture behavior of CNT-reinforced composites with different interfacial chemical bond densities. Our analysis shows that the optimal interfacial chemical bond density for (6,6) CNTs is about 5%~10% and that increasing the CNT length beyond 100 nm does not further improve fracture toughness, but can easily lead to the self-folding and clustering of the CNTs. The proposed theoretical model is also applicable to short fiber reinforced composites.

Keywords:

CNT-reinforced composites; fracture toughness; bridging effect; multi-scale simulation.