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A Homogenized Mechanical Model of Carbon Nanotubes/Polymer Composite with Interface Debonding

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Abstract : Carbon nanotubes (CNTs) possess attractive properties, such as high stiffness and strength, and high thermal and electrical conductivities, making them promising filler in multifunctional nanocomposites. Although CNTs can be efficient reinforcements, the expected level of mechanical performance of CNT-polymers is not often reached in practice due to the poor mechanical behavior of the CNT-polymer interfaces. It is believed that the interactions of CNT and polymer mainly result from the Van der Waals force. The interface debonding is a fracture and delamination phenomenon. Thus, the cohesive zone modeling (CZM) is deemed to give good capture of the interface behavior. The detailed, cohesive zone modeling provides an option to consider the CNT-matrix interactions, but brings difficulties in mesh generation and also leads to high computational costs. Homogenized models that smear the fibers in the ground matrix and treat the material as homogeneous are studied in many researches to simplify simulations. But based on the perfect interface assumption, the traditional homogenized model obtained by mixing rules severely overestimates the stiffness of the composite, even comparing with the result of the CZM with artificially very strong interface. A mechanical model that can take into account the interface debonding and achieve comparable accuracy to the CZM is thus essential. The present study first investigates the CNT-matrix interactions by employing cohesive zone modeling. Three different coupled CZM laws, i.e., bilinear, exponential and polynomial, are considered. These studies indicate that the shapes of the CZM constitutive laws chosen do not influence significantly the simulations of interface debonding. Assuming a bilinear traction-separation relationship, the debonding process of single CNT in the matrix is divided into three phases and described by differential equations. The analytical solutions corresponding to these phases are derived. A homogenized model is then developed by introducing a parameter characterizing interface sliding into the mixing theory. The proposed mechanical model is implemented in FEAP8.5 as a user material. The accuracy and limitations of the model are discussed through several numerical examples. The CZM simulations in this study reveal important factors in the modeling of CNT-matrix interactions. The analytical solutions and proposed homogenized model provide alternative methods to efficiently investigate the mechanical behaviors of CNT/polymer composites.

Keywords : carbon nanotube, cohesive zone modeling, homogenized model, interface debonding
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