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Multiscale modeling of graphite plain-weave composites with a SWNT-reinforced epoxy matrix

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Abstract

The objective of this study is to develop a multiscale modeling approach to predict the influence of molecular structure and microstructure on the bulk-level properties of a graphite/epoxy plain-woven fabric composite in which the resin-rich regions are reinforced with carbon nanotubes. The modeling approach incorporates molecular modeling and micromechanics techniques. A parametric study shows that nanotube length has a strong influence on the predicted bulk properties for nanotubes below 100 nm long. Above 100 nm, further increases in length have a negligible impact on bulk properties. It is also shown that nanotube volume fraction has a strong impact on the axial and bending laminate properties. Furthermore, nanotube functionalization to the surrounding epoxy in the resin-rich regions of the woven composite has little impact on the overall performance of the composite.

1. Introduction

Times New Roman considerable attention in recent years on account of their increased damage tolerance with respect to unidirectional and angle-ply composite laminates and because of the relative ease and low cost of fabrication of composite structures made from woven fabric pre-pregs. Woven-fabric composites are formed by the process of interlacing two individual fiber bundles or tows perpendicular to one another and impregnating with a matrix to form a single layer. As a result of the architecture of these composites, matrix-rich regions are formed in the gaps between the interlaced fiber bundles. These regions, where cracks can easily initiate and propagate, are difficult to reinforce with traditional microscale reinforcement. It has been suggested that carbon nanotubes are ideal candidates for reinforcing these resin-rich interlaminar regions because of their size and outstanding mechanical properties (Bekyarova *et al*., 2007; Garcia *et al*., 2008). In order to test this hypothesis in an efficient manner, multiscale computational modeling can be used to perform parametric studies on the expected mechanical response of these materials as a function of material geometry.

The objective of this study was to develop a multiscale modeling approach to predict the influence of molecular structure and microstructure on the bulk-level properties of a graphite/epoxy plain-woven fabric composite in which the epoxy is reinforced with single-walled carbon nanotubes (SWNTs). A recently developed molecular modeling approach (Odegard *et al*., 2005; Odegard *et al*., 2003) was used to establish the effective properties of the SWNT-reinforced epoxy matrix material that was used as an input into the fiber-undulation

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