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Modeling the Molecular Structure of the Carbon Fiber/Polymer Interphase for Multiscale Analysis of Composites

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Abstract

The carbon fiber/polymer matrix interphase region plays an important role in the behavior and failure initiation of polymer matrix composites and accurate modeling techniques are needed to study the effects of this complex region on the composite response. This paper presents a high fidelity multiscale modeling framework integrating a novel molecular interphase model for the analysis of polymer matrix composites. The interphase model, consisting of voids in multiple graphene layers, enables the physical entanglement between the polymer matrix and the carbon fiber surface. The voids in the graphene layers are generated by intentionally removing carbon atoms, which better represents the irregularity of the carbon fiber surface. The molecular dynamics method calculates the interphase mechanical properties at the nanoscale, which are integrated within a high fidelity micromechanics theory. Additionally, progressive damage and failure theories are used at different scales in the modeling framework to capture scale-dependent failure of the composite. Comparisons between the current molecular interphase model and existing interphase models and experiments demonstrate that the current model captures larger stress gradients across the material interphase. These large stress gradients increase the viscoplasticity and damage effects at the interphase which are necessary for improved prediction of the nonlinear response and multiscale damage in composite materials.

Keywords

A. Polymer-matrix composites (PMCs); B. Interface/interphase; B. Carbon fibre; C. Multiscale modelling.

1. Introduction

Polymer composites, typically containing a polymer matrix and inorganic components (additives), are ubiquitous in industrial applications and daily life. The applications of polymer composites range from consumer products to structural materials. A major barrier limiting the applications of composites is a lack of confidence in the assessment of safety and reliability of these structures under service