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A new multiscale numerical characterization of mechanical properties of graphene-reinforced polymer-matrix composites

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Abstract: In the present study, a three-dimensional multiscale simulation method for analyzing the mechanical properties of graphene-reinforced polymer-matrix composites is proposed. The macroscopic and the atomistic scales are combined in the proposed finite element modeling approach. The macroscopic homogeneous isotropic model of the matrix and the interface is included in the representative volume element (RVE) of the composites. In the nanoscale analysis, a space frame structure of graphene is selected, the carbon atoms are described as nodes, and the carbon-carbon (C-C) covalent bonds are represented with nanoscale beams. The effect of graphene volume fraction and different inclined angles on the mechanical properties of the composites is investigated under axial tension. The simulation results showed that with the increase in the graphene volume fraction, the Young's modulus and shear modulus of the graphene-reinforced composites were increased significantly. The stress transfer in the interface of the composites was also analyzed using this multiscale approach.

Keywords: Graphene; Polymer-matrix composites; Multiscale modeling; Mechanical properties; Finite element analysis

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