A Semi-Continuum Multiscale Model of Graphene Polymer Nanocomposites: Mechanical Characterization

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Abstract

The interest in polymeric nanostructured materials has been growing ever since their successful application became a sensible reality. Yet, capturing their performance using computational methods necessitates coupling between different scales and the consideration of underlying heterogeneities to ensure fidelity. For this purpose, we present a three-phases hierarchical multiscale Finite Element based model that aims to efficiently predict the mechanical behavior of graphene reinforced polymer nanocomposites. First, a discrete model of graphene is constructed using linear beam finite elements which mimic the interatomic interactions occurring at the level of the nanofiller's microstructure. The mechanical properties of graphene are then computed for several sizes to eliminate size-effects. Next, the polymer/graphene interphase is represented by non-linear spring elements which resemble van der Waals interactions occurring between the host polymer matrix and the nanofiller. With the matrix represented as a continuum, Young's modulus and Poisson's ratio of the designed polymer nanocomposite are computed by performing tensile testing in all three Cartesian directions. The semi-continuum three-phases multiscale model traversing nano to macro scales is compared against other models in the literature where it shows accuracy and efficiency in computational material modeling.

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