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Multiscale modeling of the elastic moduli of CNT-reinforced polymers and fitting of efficiency parameters for the use of the extended rule-of-mixtures

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Highlights

- An atomistic-based FEM is used in conjunction with a micromechanics approach
- Analytical and numerical micromechanics approaches are compared
- The elastic moduli of equivalent fibers are provided for numerous SWCNTs and MWCNTs
- Efficiency parameters have been fitted by polynomial expressions

Abstract

In this work, a bottom-up multiscale modeling approach is developed to estimate the effective elastic moduli of Carbon NanoTube (CNT)-reinforced polymer composites. The homogenization process comprises two successive steps, including an atomistic-based computational model and a micromechanics approach at the nano- and micro-scales, respectively. Firstly, the atomistic-based finite element model defines a cylindrical Representative Volume Element (RVE) that accounts for a carbon nanotube, the immediately surrounding matrix, and the CNT/polymer interface. The carbon-carbon bonds of the CNT are modeled using Timoshenko beams, whilst three-dimensional solid elements are used for the surrounding matrix. Through the application of four loading conditions, the RVEs are homogenized into transversely isotropic equivalent fibers by equating the associated strain energies. Secondly, the equivalent fibers are employed in a micromechanics approach to estimate the macroscopic response of non-dilute composites. This is performed using both the analytical Mori-Tanaka model and a computational RVE model with a hexagonal packing geometry. A wide spectrum of single- and multi-walled carbon nanotubes are studied, as well as two different polymeric matrices. Furthermore, the so-called efficiency parameters, imperative for the application of the simplified extended rule of mixtures, are characterized by polynomial expressions for practical filler contents. Finally, detailed parametric analyses are also provided to give insight into the sensitivity of the macroscopic response of CNT-reinforced polymer composites to microstructural features such as filler volume fraction, chirality or aspect ratio.

Keywords: Atomistic-based continuum, Carbon nanotube, Micromechanics, Mori-Tanaka method, Multiscale modeling

1. Introduction

Carbon NanoTubes (CNTs) have attracted widespread attention from the scientific community since its discovery in the '90s [1]. Due to their exceptional mechanical and physical properties, as well as their high aspect ratio and low mass density [2–5], very low filler dosages provide outstanding improvements in the overall response of CNT-based composites. Moreover, CNTs also exhibit remarkable electrical and self-sensing properties [6], which open a vast spectrum of applications for the development of multi-functional and smart composites [7–9]. Hence, accurate quantification of the material properties of CNT-reinforced composites is of pivotal importance for their design and optimization. Notwithstanding many efforts have been made from experimentation, today, the synthesis of CNT nanocomposites demands the use of complex processing methods and sophisticated testing equipment, what results in exorbitant costs [10]. Conversely, computational modeling offers a flexible and efficient alternative for predicting the properties of CNT/polymer composites and assisting their design [11, 12].

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