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A coarse-grained model for the elastic properties of cross linked short carbon nanotube/polymer composites

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Abstract

Short fiber reinforced polymer composites have found extensive industrial and engineering applications owing to their unique combination of low cost, relatively easy processing and superior mechanical properties compared to their parent polymers. In this study, a coarse-grained (CG) model of cross linked carbon nanotube (CNT) reinforced polymer matrix composites is developed. A characteristic feature of the CG model is the ability to capture the covalent interactions between polymer chains, and nanotubes and polymer matrix. The dependence of the elastic properties of the composites on the mole fraction of cross links, and the weight fraction and distribution of nanotube reinforcements is discussed. The simulation results reveal that the functionalization of CNTs using methylene cross links is a key factor toward significantly increasing the elastic properties of randomly distributed short CNT reinforced poly (methyl methacrylate) (PMMA) matrix. The applicability of the CG model in predicting the elastic properties of CNT/polymer composites is also evaluated through a verification process with a micromechanical model for unidirectional short fibers.

Keywords: Polymer-matrix composites (PMCs), Carbon fibre, Mechanical properties, Computational modelling

1. Introduction

Short fiber reinforced polymer (SFRP) composites have attracted intense attention due to their ease of fabrication, low manufacturing costs and superior mechanical, thermal and

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