



Graphene reinforced nanocomposites: 3D simulation of damage and fracture



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ABSTRACT

3D computational model of graphene reinforced polymer composites is developed and applied to the analysis of damage and fracture mechanisms in the composites. The graphene/polymer interface properties are determined using the inverse modeling approach. The effect of composite structure, in particular, of the aspect ratio, shape, clustering, orientation and volume fraction of graphene platelets on the mechanical behavior and damage mechanisms of nanocomposites are studied in computational experiments. It was shown that the Young modulus of the nanocomposites increases with increasing aspect ratio, volume content, elastic properties of graphene/polymer interface layer, and decreasing the degree of intercalation. The tensile strength follows similar tendencies, except for the aspect ratio and clustering degree, where the opposite effects are observed. Nanocomposites with randomly oriented sheets of graphene demonstrate much lower Young modulus and strength as compared with the composites with the aligned graphene sheet reinforcement. It was further concluded that the structural imperfections of graphene reinforcement (like crumpling shape or random misalignment) have considerable effect on the composite performances.

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1. Introduction

Graphene, a strong and light two-dimensional allotrope of carbon, attracted a growing interest of research community and industry in recent years [1–3]. Graphene sheets can be used, among others, as reinforcement in polymer composites, thus, potentially ensuring a drastic improvement of properties of the composites [4,5].

In order to explore the potential of graphene nanoreinforcements for the polymer strengthening, and to develop recommendations for the computational design of the composites, computational models linking microstructures of graphene reinforced composites with their mechanical properties and strength are necessary. A number of computational models of graphene sheets and graphene reinforced composites have been developed in recent years.

Many models are based on atomistic, combined atomistic-continuum (FE) and nanoscale-continuum approaches [1,10–12]. A detailed review of the methods of modeling of graphene and graphene based composites including Quantum Chemistry, molecular dynamics, Monte Carlo simulation and other techniques has been published by Zhang et al. [13]. Quite often, molecular dynamics (MD) simulations are employed to analyze the properties of

graphene sheets and their interaction with polymer matrix. Zhang and Gu [14] used molecular dynamics simulations to determine elastic modulus, fracture stress and fracture strain of graphene. They demonstrated that mechanical properties of graphene are much more sensitive to the temperature changes than to the layer numbers in the multilayer graphene. Li et al. [15] also used MD simulations to characterize multilayer graphene reinforced epoxy composites. They considered two configurations (graphene layers parallel and perpendicular to polymer/graphene interface), and have shown that the strengths of composites are close in both cases, while the damage mechanisms can be different: “the parallel case exhibits cohesive yield with strain localization and nano-void formation within the bulk polymer while the case with graphene sheets oriented normal to the interface exhibit interfacial debonding”. Shiu and Tsai [16] used molecular dynamics simulations, to evaluate mechanical properties of graphene reinforced nanocomposites with different morphologies (graphene platelets, intercalated graphene and intercalated graphene oxide). It was shown that the composites with intercalated graphene have a higher Young’s modulus, than do those with graphene platelets. The graphene oxide was shown to be the best reinforcement of the three considered cases. Molecular dynamics approach can deliver rather detailed information on the deformation and damage mechanisms at the nanoscale. On the other side, the continuum mechanics/finite element (FEM) based approaches can be efficiently used

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