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Characterization of graphene epoxy nanocomposite interface region by multiscale modelling

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Abstract

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The aim of this study was to characterize graphene epoxy nanocomposite interfacial region using multiscale modelling. Molecular dynamics was used to study the nanocomposite at nano scale and finite element analysis at macroscale to complete the multiscale modeling. Coupling of these two scales was done by the use of a property averaging method known as Irving Kirkwood method. One to three sheets (1.8 %, 3.7 % and 5.4 % graphene weight fraction) of graphene were respectively reinforced with epoxy polymer to form a graphene epoxy nanocomposite. The normal and shear forces at the interfacial region of graphene epoxy nanocomposite were investigated by displacing graphene from epoxy to analyze the mechanical properties including the Youngs Modulus, shear modulus and traction forces. Molecular dynamics simulations were further studied through radial distribution function and molecular energy. The effects of graphene on the density distribution of epoxy in the nanocomposites were also analyzed. The results showed that the density when graphene is added sheet by sheet relatively increases until saturation, and then progressively decreases to a bulk value in regions further away from the interface. Improvements in Youngs Modulus and shear modulus of graphene epoxy model compared to normal epoxy resin were noticed. The dispersed graphene sheet improved the Elastic Modulus more than the agglomerated graphene sheets. The normal and shear forces versus displacement were plotted in order to characterize the interfacial region properties. The elastic constants determined by molecular dynamics were higher than those predicted at macroscale analysis due to the difference in scales. The nanocomposite with 3.7 % weight fraction of graphene gave the best properties of the interfacial region. The results from this model also showed close agreement with the available numerical experiments results from the literature data.

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