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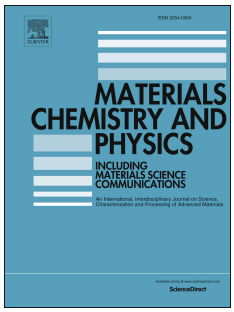

Combining density functional theory-finite element multi-scale method to predict mechanical properties of polypropylene/graphene nanocomposites: Experimental study

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Combining density functional theory- finite element multi-scale method to predict mechanical properties of polypropylene/graphene nanocomposites: Experimental study

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Abstract

In this paper a multi-scale finite element model is developed to study the tensile modulus of graphene reinforced polypropylene (PP/graphene) nanocomposites and compare the results with experimental tensile tests. Herein, the graphenes are modeled and optimized using density functional theory (DFT). By treating graphene as space-frame structures, in which the discrete nature of graphene is preserved, they are modeled using three-dimensional elastic beam elements for the C-C covalent bonds and point mass elements for the atoms. Our calculations reveal that the force constants of stated elastic beam obtained from DFT method are in best agreement comparing to the results of previous MD study which was equal to k_r=6.41 ×10^{-7} N/nm, k_θ=8.47×10^{-10} N.nm/rad^2 and k_τ=2.7×10^{-7} N.nm/rad^2. The interlayer van der Waals forces between graphene and PP matrix are represented by Lennard–Jones potential and simulated by a nonlinear truss rod model. According to our DFT results we found that interaction energy between graphene and PP matrix decreased by increasing in the number of polymer matrix monomers and reached to a constant value when six monomer of polymer adsorbed onto the surface of graphene which was equal to -0.0044 eV/monomer. Our FE results showed that the moduli of the nanocomposites were close to the experimental results until 1 wt% of graphene and also were predictable. The Young's modulus obtained from combined model and experimental test were about 2.85 Mpa and 2.21 Mpa for 0.25 wt%, 3.88 Mpa and 3.22 Mpa for 0.5 wt%, 4.83 Mpa and 4.30 Mpa for 0.75 wt% and also 5.86 Mpa and 5.19 Mpa for 1 wt% of graphene, respectively.

Keywords:

Polypropylene; Graphene; DFT; Multi-scale; Mechanical Properties

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