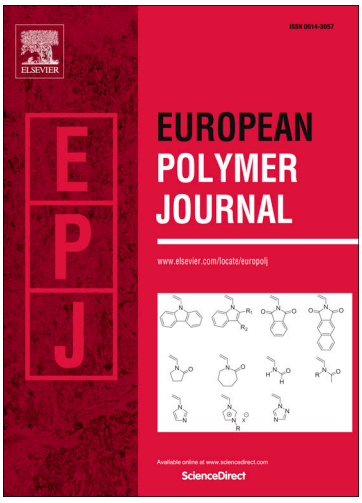

Tensile behavior of polymer nanocomposite reinforced with graphene containing defects

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Tensile behavior of polymer nanocomposite reinforced with graphene containing defects

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Abstract: This paper investigates the tensile behavior in both armchair and zigzag directions of polymer nanocomposites reinforced with defective single layer graphene containing single or double vacancies by using molecular dynamics simulations. The results show that the overall material properties including Young's modulus, ultimate strength and strain in both directions decrease with an increasing number of missing atoms but are insensitive to defect distribution. Compared with double-vacancy, single-vacancy defects have a more significant influence on the material properties due to more dangling bonds in its structure. In addition, it is found that the defect type, size and location also play an important role in the mechanical properties of the nanocomposite. The mechanism of these defect parameters underlying the tensile behavior of graphene reinforced epoxy nanocomposite is explored at the nanoscale.

Keywords: Graphene reinforced epoxy nanocomposite; Single vacancy; Double vacancy; Structural defect; Tensile properties; Molecular dynamics simulation

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