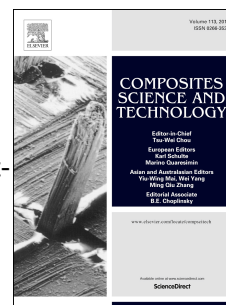


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Multiscale Multiphysical Analysis of Photo-Mechanical Properties of Interphase in Light-Responsive Polymer Nanocomposites

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Abstract

The design of the adaptive mechanical behavior of polymer nanocomposites driven by light irradiation has attracted considerable attention in the fields of physical chemistry and mechanical engineering. To assess the photo-mechanical properties of photo-responsive polymer (PRP) nanocomposites reinforced with gold nanoparticles *via* continuum mechanics, we first investigated interfacial properties of PRP nanocomposites by using a novel multiscale multiphysical model. Particularly, the interfacial interactions between the nanoparticle and polymer matrix under external loading were addressed by combining all-atom molecular dynamics (MD) simulations with finite element (FE) analysis. To explicitly characterize the role of the interfacial interactions between the nanoparticle and polymer matrix in strain energy density under photo-mechanical loading, the effective stiffness and the spatial range of the interphase layer were numerically identified by matching the deformation energy in the FE model with that in the MD model using the energy method and the homogenization theory. It is verified that the equivalent continuum model obtained by the multiscale method satisfactorily predicts not only the overall mechanical properties of nanocomposites, but also the local stress distribution at the interphase as well as the inherent nanoparticle size and photo-isomerization reaction effects of the nanocomposites. The present multiscale analysis reveals that the effective interfacial region around the nanoparticle is considerably weakened as the photo-isomerization reaction progresses, as well as the decrease of the thickness of the interfacial region.

Keywords: A. Smart Materials; A. Nano composites; B. Interphase; C. Computational mechanics

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