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Multiscale modeling of photomechanical behavior of photo-responsive nanocomposite with carbon nanotubes

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Abstract

We propose a scale-bridging methodology to link the microscopic photoreaction of an azobenzene-containing liquid crystalline polymer (LCP) and the macroscopic interfacial and elastic properties of carbon nanotube (CNT)-reinforced photo-responsive nanocomposites. The photo-isomerization of the azobenzene moieties is described by implementing a photo-switching potential that represents the light-excited energy transition path. The relevant time evolution of the molecular shape and the concurrent changes in the interfacial morphology are observed using molecular dynamics (MD) simulations. Finally, the effective elastic properties of the photo-responsive polymer (PRP) nanocomposite with respect to the isomerization ratio are numerically derived using the micromechanics-based homogenization method. It is verified that the size of the CNT and the photo-deformation of the azobenzene molecules influence the intermolecular interactions and the nematic phase of the LCP at the interfacial region. The continuum-scale finite element (FE) model, which reflects the microscopic information, clearly predicts the reinforcing effect of the CNT filler on the elastic properties of the composite and their variation under photo-actuation. We expect our results to shed light on designing the photomechanical energy conversion efficiency of nano-sized soft actuators composed of CNT-reinforced composites.

Keywords: Multiscale modeling, Nanocomposite, Carbon nanotube, Liquid crystalline polymer, Photomechanics

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