Accepted Manuscript

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

Junghwan Moon, Hyunseong Shin, Kyungmin Baek, Joonmyung Choi, Maenghyo Cho

PII: S0266-3538(17)32726-4

DOI: 10.1016/j.compscitech.2018.03.032

Reference: CSTE 7150

To appear in: *Composites Science and Technology*

Received Date: 31 October 2017

Revised Date: 21 March 2018

Accepted Date: 22 March 2018

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

Junghwan Moon[a], Hyunseong Shin[b], Kyungmin Baek[a], Joonmyung Choi[a c], Maenghyo Cho[a c,*]

[a]*Department of Mechanical and Aerospace Engineering, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Republic of Korea*

[b]*School of Mechanical Engineering, Yeungnam University, 280 Daehak-ro, Gyeongsan, Gyeongbuk 38541, Republic of Korea*

[c]*Institute of Advanced Machines and Design, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, Republic of Korea*

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

[*] Corresponding author: Tel.: +82-2-880-1693, Fax: +82-2-886-1645.
E-mail address: mhcho@snu.ac.kr