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The Effect of Elongational Flow on the Placement and Orientation of Nanorods in Polymer: Modeling and Experiments JAY PARK, Cornell University, VIBHA KALRA, Drexel University, YONG JOO, Cornell University — Nanorods are often incorporated into a polymer to enhance its functionality. Gaining control over the placement of nanorods in polymer is important to improve the desired nanocomposite material property and for application like solar cell. First, we used coarse-grained molecular dynamics (CGMD) simulation to quantitatively examine the effect of elongational flow on the placement of model nanorods in homopolymer matrix. We have investigated how flow strength, concentration, interaction, and aspect ratio of nanorods affect its placement in homopolymer. As an analogous experiment, we have electrospun polyvinyl alcohol (PVA) in water with Au nanorods. The experimental result showed dispersion and alignment of Au nanorods, as predicted by the simulation. We also demonstrated selective placement of nanorods along the outer layer of fiber by co-axially electrospinning PVA/Au nanorods and pure PVA as shell and core, respectively. The material properties of the PVA/Au nanocomposite fiber are tested to show its potential application such as electromagnetic interference (EMI) shielding. The good agreements between simulation and experiment suggest that CGMD simulation can be used as a predictive tool for controlling nanorod placement in a polymer under extensional flow.

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