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Slip-spring model of entangled rod-coil block copolymers

MUZHOU WANG, National Institute of Standards and Technology, ALEXEI E. LIKHTMAN, University of Reading, BRADLEY D. OLSEN, Massachusetts Institute of Technology — Understanding the dynamics of rod-coil block copolymers is important for optimal design of functional nanostructured materials for organic electronics and biomaterials. Recently, we proposed a reptation theory of entangled rod-coil block copolymers, predicting the relaxation mechanisms of activated reptation and arm retraction that slow rod-coil dynamics relative to coil and rod homopolymers, respectively. In this work, we introduce a coarse-grained slip-spring model of rod-coil block copolymers to further explore these mechanisms. First, parameters of the coarse-grained model are tuned to match previous molecular dynamics simulation results for coils, rods, and block copolymers. For activated reptation, rod-coil copolymers are shown to disfavor configurations where the rod occupies curved portions of the entanglement tube of randomly varying curvature created by the coil ends. The effect of these barriers on diffusion is quantitatively captured by considering one-dimensional motion along an entanglement tube with a rough free energy potential. Finally, we analyze the crossover between the two mechanisms. The resulting dynamics from both mechanisms acting in combination is faster than from each one individually.

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