Dynamics in Model Microphase Separated Tapered Copolymers[1]

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— Microphase separating copolymer systems are of interest in transport and separation applications because one can take advantage of the different properties of two different monomer types. For typical AB diblock copolymers, the main control parameters that set the structure and properties are the monomer-monomer interactions and the fraction of A monomers; one can further control both structure and dynamics by modifying the sequence of A and B along the chain. Here we consider how adding a tapered midblock between pure A and B blocks impacts the dynamics of the chains and of added monomer-sized penetrants that are selectively solvated by the A microphase. Specifically, we perform coarse-grained molecular dynamics simulations of linear, fully flexible, symmetric polymers, and the tapered region has a linear gradient in composition from pure A to pure B (or from pure B to pure A for an inverse taper); we also consider systems with a random midblock for comparison. As the length of the normal taper increases, the diffusion constant of both polymers and penetrants parallel to the lamellae increases. In contrast, the diffusion constant of inverse tapered chains is non-monotonic as a function of taper length. We show how different types of polymer conformations contribute to this trend.

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