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Molecular Dynamics Simulations of Microphase Separating Tapered Diblock Copolymers YOUNGMI SEO, JONATHAN R. BROWN, LISA M. HALL, The Ohio State University — Tapered AB copolymers consist of pure A and B blocks separated by a middle block whose composition is a statistical linear gradient from pure A to pure B (or from B to A for an inverse taper). These systems microphase separate into ordered structures similar to typical AB diblock copolymers. Prior experiments and theory suggest that one can use taper length as an adjustable parameter (beyond those available in the diblock system) to control interfacial and phase behavior, and that tapers potentially make the bicontinuous double gyroid phase more accessible at high molecular weight. Using a simple coarse-grained model, we perform molecular dynamics (MD) simulations to determine the interfacial profiles and other features of the structure and dynamics as a function of taper length. We reproduce the results from self-consistent field theory (SCFT); specifically, tapering increases miscibility, widens the interfacial region, shortens domain spacing, and makes network phases more preferable. The significantly smaller lamellar spacing for inverse tapers is explained in terms of polymer chain folding or snaking across the interface The dynamic analysis shows the diffusion and relaxation behavior are closely related to the chain conformations and interfacial behavior. The effect of tapering on penetrant diffusion through one of the microphases will also be discussed.

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