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Microphase Separation and Interfacial Behavior of Model Tapered Diblock Copolymers LISA M. HALL, YOUNGMI SEO, JONATHAN R. BROWN, The Ohio State University — We use a combination of theoretical and simulation methods to understand the microphase separated structure and dynamics of model copolymers. Tapered diblock copolymers, containing pure A and B blocks separated by a region with an A/B composition gradient, are of particular interest: the length of the tapered region can be adjusted to modify the system's phase and interfacial behavior. Experimentally, tapered diblocks have been found to form the bicontinuous gyroid phase, which is of interest for transport applications and can be difficult to access using typical diblocks. Phase diagrams from self-consistent field theory (SCFT) do show a larger gyroid region for certain tapered systems versus diblocks. To further understand the detailed microphase separated structure, we employ fluids density functional theory (fDFT) and molecular dynamics (MD) simulations together. These both capture monomer scale packing effects and are implemented for very similar models so that the fDFT results can be used as a guide to ensure the appropriate equilibrium state is formed in the MD simulations. Density profiles from SCFT, fDFT, and MD are in qualitative and sometimes quantitative agreement; tapers widen the interfacial region and large tapers decrease the maximum purity of the microphases.

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