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Morphology and Dynamics of Tapered Diblock Copolymers from fDFT-initialized MD Simulations LISA M. HALL, YOUNGMI SEO, JONATHAN R. BROWN, The Ohio State University — Tapered block copolymers are similar to AB diblock copolymers, but with a statistical A-to-B (normal) or B-to-A (inverse) gradient "taper" between the A and B blocks. Depending on the sequence of monomers along the chain and the segregation strength, the A and B monomers are known to microphase separate into various ordered morphologies. Tapering introduces an additional parameter, independent of molecular weight or polymer choice, to tune morphology, and has been shown previously to widen the gyroid region of the phase diagram.In this study, we use classical, fluids density functional theory (fDFT) and molecular dynamics (MD) simulations to study the morphology and dynamics of tapered systems. Using fDFT allows us to accurately compare free energies between different potential microphases as a function of interaction parameter and fraction of A. Because of the similarity of the fDFT and MD models, the fDFT results map very closely with the corresponding MD model. We use the fDFT density profiles to generate the initial state of the chains for the simulations. Lamellae, cylinders, and other phases can be generated in this way with approximately correct spacing and density. We apply the streamlined simulation setup to analyze the effect of tapering on conformations and dynamics.

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