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Theory and Simulations of Tapered Diblock Polymers[1] LISA M. HALL, YOUNGMI SEO, JONATHAN R. BROWN, The Ohio State University — We study tapered block polymers, AB diblock polymers with a gradient region inserted between the pure A and B blocks such that composition smoothly transitions from A to B (or B to A in the case of inverse tapers). Phase diagrams were created using self consistent field theory (SCFT), and coarse-grained molecular dynamics (MD) simulations were used to study polymer conformations and diffusion, including diffusion of monomer-sized penetrants preferentially dissolved in one of the phases. As has been observed experimentally, we find that tapering makes the A and B blocks more miscible, decreasing domain spacing and shifting the order to disorder transition to lower temperatures. We predict a widening of the bicontinuous double gyroid region of the phase diagram for moderate length normal tapers versus diblocks, suggesting taper length can be used as a control parameter to obtain network phases even at high molecular weight, as may be desirable in transport applications. Additionally, in some inverse tapered systems, SCFT predicts phases not present in the standard AB diblock phase diagram, and MD simulations show how the chains fold back and forth across the interface. In these inverse tapered polymers, as segregation strength is increased, the competing effects of folding and stretching produces lamellae that have domain spacing nearly independent of temperature. We also find that diffusion of penetrants in normal tapers is significantly faster than that in inverse tapers, which is likely related to their unusual conformations.

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