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Simulation of chain diffusion in diblock copolymer microstructures using dynamical self-consistent mean-field theory DOUGLAS GRZETIC, ROBERT WICKHAM, University of Guelph — We simulate chain diffusion in ordered phases of a diblock copolymer melt, using our recently-developed dynamical self-consistent mean-field theory [*J. Chem. Phys.* **140**, 244907 (2014)]. This theory enables us to study large length and time scales in these dense systems, while remaining connected, in a self-consistent manner, to the microscopic physics of Brownian chains whose beads interact via a species-dependent modified Lennard-Jones potential. In the LAM and HEX phases, chain diffusion perpendicular to the microdomain interface is exponentially suppressed with increasing segregation, while parallel diffusion is unaffected. In the BCC phase, diffusion is isotropic and is gradually suppressed with increasing segregation. Chain diffusion is also isotropic in the gyroid phase, but does not vanish with increasing segregation. Instead, the diffusion constant asymptotes to a value consistent with chain diffusion being restricted to the interface of the three-dimensional gyroid network of struts, characterized by a network tortuosity value of 1.72. Finally, we measure the out-of-equilibrium evolution of the anisotropy in the chain diffusion as metastable LAM transforms to stable HEX over long times.

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