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Molecular Dynamics Simulations of Penetrants in Microphase Separated Tapered Diblock Copolymers[1] YOUNGMI SEO, JONATHAN R. BROWN, LISA M. HALL, Ohio State Univ - Columbus — Tapered AB diblock copolymers contain pure A and B monomer blocks on the ends with a tapered midblock of intermediate composition, providing taper length as an additional tuning parameter to control microphase separation and interfacial behavior. We model the midblock as a statistical linear gradient from pure A to pure B. Recent experiments with salt dissolved in one of microphases show that a certain length of taper increases ion conductivity while the same length of inverse taper lowers conductivity. We perform coarse-grained molecular dynamics simulations of tapered copolymers with monomer sized penetrants, which have preferential interactions with one microphase, to better understand this observation and the general effects of tapering on dynamics. We calculate penetrant diffusion, polymer relaxation times, and other quantities over the range from 0% (diblock) to 100% (full gradient) taper length, with the taper direction either normal or inverse (with the A side of the taper connected to the pure B block). Normal taper results typically lie between those of diblocks and full gradients, while inverse tapers show strong nonmonotonic behavior as a function of taper length. For intermediate length inverse tapers, penetrant and monomer dynamics are significantly slower than those of diblocks or normal tapers, and this relates to the folding of the inverse chains back and forth across the interface. To provide further insight, we also compare to the dynamics of random copolymers of various compositions.

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