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Connecting Molecular Dynamics Simulations and Fluids Density Functional Theory of Block Copolymers[1]

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Increased understanding and precise control over the nanoscale structure and dynamics of microphase separated block copolymers would advance development of mechanically robust but conductive materials for battery electrolytes, among other applications. Both coarse-grained molecular dynamics (MD) simulations and fluids (classical) density functional theory (fDFT) can capture the microphase separation of block copolymers, using similar monomer-based chain models and including local packing effects. Equilibrium free energies of various microphases are readily accessible from fDFT, which allows us to efficiently determine the equilibrium nanostructure over a large parameter space. Meanwhile, MD allows us to visualize specific polymer conformations in 3D over time and to calculate dynamic properties. The fDFT density profiles are used to initialize the MD simulations; this ensures the MD proceeds in the appropriate microphase separated state rather than in a metastable structure (useful especially for nonlamellar structures). The simulations equilibrate more quickly than simulations initialized with a random state, which is significant especially for long chains. We apply these methods to study the interfacial behavior and microphase separated structure of diblock and tapered block copolymers. Tapered copolymers consist of pure A and B monomer blocks on the ends separated by a tapered region that smoothly varies from A to B (or from B to A for an inverse taper). Intuitively, tapering increases the segregation strength required for the material to microphase separate and increases the width of the interfacial region. Increasing normal taper length yields a lower domain spacing and increased polymer mobility, while larger inverse tapers correspond to even lower domain spacing but decreased mobility. Thus the changes in dynamics with tapering cannot be explained by mapping to a diblock system at an adjusted effective segregation strength.

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