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Study of Self-Assembly in Block Copolymer (BCP)-Homopolymer Blends using Dissipative Particle Dynamics (DPD) Simulations AMY GOODSON, MD FAKAR UDDIN, JULIE ALBERT, Tulane Univ — We demonstrate the use of Dissipative Particle Dynamics (DPD) simulations to study self-assembly behavior of block copolymer (BCP) melts and BCP-homopolymer blends. DPD is a coarse-grained simulation technique that preserves hydrodynamics, thereby allowing simulations to capture not only equilibrium conformations but also understand the pathways by which they form. DPD simulations of pure A-block-B melts conducted at varying f and chi*N produce a phase diagram that mimics the trends seen experimentally and in Self-Consistent Field Theory (SCFT). These simulations also reproduce expected domain spacing relationships with chi*N. DPD simulations of BCP-homopolymer blends match results obtained experimentally in our group. As homopolymer is added to a symmetric BCP, lamellar domain spacing swells. At a critical homopolymer content, the lamellar structure is lost and a non-symmetric, bicontinous microstructure forms. We also examine the relationship of block and homopolymer molecular weights and the microstructure observed in the blend.

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