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Dynamical self-consistent field theory of the evolution of instabilities in polymer blends and diblock copolymer melts DOUGLAS GRZETIC, ROBERT WICKHAM, Univ of Guelph — We demonstrate our recently-developed dynamical self-consistent mean-field theory [J. Chem. Phys. 140, 244907 (2014)] in a polymeric context, by studying the early-time spinodal decomposition of a symmetric binary polymer blend and the dynamics of the order-order transition between the LAM and HEX phases in an asymmetric diblock copolymer melt. A Brownian dynamics description of a dense system of Rouse chains interacting pair-wise via a modified, species-dependent Lennard-Jones potential is reformulated, through a novel dynamical mean-field approximation, as that of a single chain interacting with a self-consistently determined dynamical mean force-field. A large ensemble of single chain Brownian dynamics simulations, run in parallel, efficiently determines the space- and time-dependent density that is used to weight the Lennard-Jones interaction in the mean force-field calculation. Our theory gives access to chain conformation statistics, maintains a connection to microscopic time-scales and scales favorably with chain-length via a fast Rouse transform. We examine the performance of our method, and discuss our results for the growth of unstable modes in the blend and in the diblock copolymer melt.

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