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Coarse-Graining in Simulations of Multicomponent Polymer Systems VAIDYANATHAN SETHURAMAN, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin, Austin, Texas 78712, USA — We investigate the mapping required between the interaction parameters of two different coarse-grained simulation models to ensure a match of the long-range structural characteristics of multicomponent polymeric system. We investigate the extensibility of mapping functions deduced in the context of symmetric block copolymers by Morse and coworkers to other polymeric systems by studying a variety of systems, including, asymmetric diblock copolymers, symmetric triblock copolymers and diblock copolymer-solvent mixtures. We observe excellent agreement for peak in the inverse structure between two popular coarse grained models for all sets of polymeric melt systems investigated, thus showing that the mapping function proposed for diblock copolymer melts is transferable to other polymer melts irrespective of the blockiness or overall composition. We use our findings to propose a methodology to create ordered morphologies in simulations involving hard repulsive potentials in a computationally efficient manner.

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