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Phase Behavior of Semi-flexible-Coil Block Copolymers Studied by Monte Carlo Simulations TAO WEI, ROBERT RIGGLEMAN, Department of Chemical and Biomolecular Engineering, University of Pennsylvania — Semi-flexible/coil and rod/coil polymers have attracted increasing interest in the applications of organic electronics and biomaterials due to their novel supramolecular structures with nanoscale architecture and tunable domain size. The coupling of microphase separation and liquid-crystalline ordering, stemming from chain rigidity, yields complex phase behaviors. In this work, phase morphologies and phase diagram of semi-flexible/coil block copolymers were identified with efficient Theoretical informed coarse-grained Monte Carlo (TIMC) simulations, which tracks the local density of each grid, rather than computationally demanding pair-wise interactions. Besides the common Flory-Huggins interactions between dissimilar components, we incorporate anisotropic interactions through a Maier-Saupé potential. Due to the increased complexity of semi-flexible polymer, parameter number is significantly larger compared to fully flexible polymers. We will illustrate the TIMC method for semi-flexible/coil polymers and examine fluctuation effect on various phase diagrams. We demonstrate the influence of the relative strength of Maier-Saupé parameter to Flory-Huggins parameter, as well as the geometric factors that characterize the size of the semi-flexible block relative to the coil block.

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