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Liquid crystalline order of semiflexible polymer melts and blends

KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, The University of Akron — Semiflexible polymers of sufficient stiffness exhibit liquid crystalline order at low temperature and high polymer concentration. This phenomenon is investigated with Monte Carlo simulations of a bond fluctuation lattice model, where the chain stiffness is controlled by a bending penalty for bond angles less than 180°. We observe a discontinuous transition from the high-temperature, isotropic to a low-temperature, ordered state as the chains undergo a transition from coil- to rod-like conformations. Simulation snapshots show that melts that have undergone the transition are segregated into high-density ordered and low-density disordered regions. For a full characterization of the system, we construct the phase diagram in the inverse temperature - density plane and we consider the effect of an external ordering field. To analyze the structure of ordered and disordered regions we calculate pair-distribution functions for sites on different subsets of chains. In blends of two types of polymers, one that undergoes the ordering transition and one that does not, we find interesting morphologies with domains of ordered rods embedded in disordered mixed regions.

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