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Computer simulation of the formation of random-blocky copolymers LAWRENCE STRICKLAND, JAN GENZER, CAROL HALL, North Carolina State University — A recent computational study described a new method for producing random copolymers (RCPs) with tunable monomer sequence distribution; the technique is based on adjusting the size of a homopolymer (say A) coil and performing a chemical reaction ("coloring") with certain chemical moieties (say B) on the accessible monomers of the homopolymer chain. While experimental evidence exists that can relate the comonomer distribution in the A-B copolymer to the original homopolymer dimension in the solvent, the "coloring" mechanism is difficult to reconcile as there exists competing mechanisms, involving the coloring process itself and the tendency for the copolymer to change conformation during the "coloring" driven by the changing solubility of the resultant A-B copolymer relative to that of the A homopolymer. In this work we use discontinuous molecular dynamics (DMD) to comprehend the formation of A-B copolymers. Our RCPs were constructed by reacting homopolymers in varying solvents and reactant concentrations. We show how we can selectively tune the randomness by varying chain length and system temperature. While increasing system temperature leads to formation of A-B copolymers with random distribution of segments, increasing monomer solubility leads to A-B copolymers with random-blocky co-monomer sequences.

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