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Effect of copolymer microstructure on single chain collapse ASHOK DASMAHAPATRA, Polymer Division, National Chemical Laboratory, Pune and Department of Chemical Engineering, IIT Bombay, GURUSWAMY KUMARASWAMY, Polymer Division, National Chemical Laboratory, Pune, HE-MANT NANAVATI, Department of Chemical Engineering, Indian Institute of Technology Bombay — We present dynamic Monte Carlo simulations of the collapse of copolymers containing sticky comonomers, c. There is a qualitative difference in the transition depending on c content. For c content > 0.50%, copolymer collapse is qualitatively similar to that observed for homopolymers, when rescaled to account for comonomer solvophobicity. However, collapse of copolymers with c $< ~~\sim 50\%$ is qualitatively steeper than for homopolymers. We show that the change in the nature of collapse is due to the formation of an intermediate structure after the theta-point. The pathway to collapse is also strongly influenced by the distribution of comonomers along the chain. For uniform copolymer chains (viz. equispaced cunits), collapse happens at lower temperatures than random copolymers. Further, uniform copolymers, but not random, appear to collapse cooperatively. Our results have relevance to protein folding where specific amino acid sequences lead to collapse and folding to a unique native structure.

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