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Effect of additive particles on the crystallization of homopolymers ASHOK DASMAHAPATRA, Chemical Engineering, IIT Bombay and Polymer Division, National Chemical Laboratory, Pune, India, GURUSWAMY KUMARASWAMY, Polymer Division, National Chemical Laboratory, Pune, India, HEMANT NANAVATI, Chemical Engineering, IIT Bombay, India — The effect of additive particles on polymer crystallization has been investigated using lattice dynamic Monte Carlo simulation. Additives are compatible with the polymer matrix (viz. there is an attractive "sticky" interaction between additives and monomers) and, additive particles have the same size as a monomer. Polymer crystallization is strongly influenced by both additive fraction, x and the additive-monomer interaction strength, λ. With increase in x or λ, the diffusivity of the polymer chain decreases dramatically. The decrease in chain mobility correlates with lower crystallinity and smaller crystallite sizes. Further, the presence of additive particles also dramatically suppresses the peak in specific heat during crystallization. Structural analysis shows that the additive particles are well-dispersed in the polymer matrix – they are surrounded by both crystalline and non-crystalline chain segments, the relative proportions of which depend on x and λ. We show that sticky additive particles suppress crystallization.

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