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Monte Carlo Simulations of Strain-induced Polymer Crystal Nucleation[1] WENBING HU, YIJING NIE, HUANHUAN GAO, Nanjing University, School of Chemistry and Chemical Engineering, State Key Lab of Coordination Chemistry — We performed dynamic Monte Carlo simulations of lattice polymer chains, to investigate primary crystal nucleation induced by a homogeneous stretching at high temperatures. We developed a new scheme to realize a homogeneous stretching of bulk polymer chains with their one chain ends fixed on a shifting plane and the other ends on a fixed plane. We observed a sudden decay of chain-folding probability in those newly emerged small crystallites, which indicated a transition of crystal nucleation from intramolecular mode to intermolecular mode. There exists a competition between two nucleation modes, as revealed by a theoretical fitting of the critical strains for mode transitions at various temperatures. The theoretical estimation is based on the classical nucleation theory.

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