

Abstract Submitted
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Strain-induced transition from intramolecular to intermolecular crystal nucleation¹ YIJING NIE, WENBING HU, State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, China — We performed dynamic Monte Carlo simulations of strain-induced crystallization of bulk polymer chains. We observed that for small crystallites grown at relatively high temperatures, the probabilities of adjacent chain-folding jump down at a critical strain. The result implies that polymer chains prefer to choose intramolecular crystal nucleation at small strains, and the intermolecular crystal nucleation becomes dominant only when the strain is higher than the critical value. In addition, the critical strains appear as almost constant to temperatures.

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