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Molecular dynamics simulations of polymer crystallization via self-seeding[1] CHUANFU LUO[2], JENS-UWE SOMMER, Leibniz Institute of Polymer Research Dresden, 01069, Germany — We use large scale molecular dynamics (MD) to simulate the processes of polymer crystallization with a coarse-grained model. In total we are able to simulate 1000 polymer chains made of 1000 monomers each, a system large enough to compare to experimental relevant, entangled melts. It is found that some micro crystalline domains (MCDs) can survive slightly above the apparent melting temperature after a consistent cooling and reheating cycle. We chose the stablest MCD as a baby seed and let it grow at a constant quenched temperature. A single lamella can be formed via this self-seeding process. We observe the growth pathway and analyze the chain dynamics especially at the growth front.

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