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Structure and Evolution of Ordered Domains in Deeply Quenched Polyethylene Melt NAIDA LACEVIC, LAURENCE FRIED, RICHARD GEE, Lawrence Livermore National Laboratory — Solidification of polymeric materials strongly depends on how the melt is cooled below its crystallization temperature. If cooling is at moderate rates, the most common and well understood mechanism is via nucleation and growth of spherulites, but special cases exist where crystallization is preceded by a pre-transition state induced by density fluctuations. Such multi-step crystallization scenarios are suggested by many experiments, and recent theoretical and simulation work. In this special case, the melt is quenched into a metastable region and the transition from the disordered phase to an ordered phase is uniform in contrast to the classical nucleation and growth mechanism. In this study we investigate this continuous transition. We have conducted the largest and longest timescale simulations of polyethylene to date. These elucidate the initial separation of a metastable, mesomorphic phase. Via energetic and geometric analyses, we have examined the structure of mesomorphic domains and the dynamics of their formation and evolution, including atomic scale details of molecular addition to ordered domains, as well as particle dynamics in the system, including high mobility jumps in the ordered domains at wavelengths matching the monomer spacing.

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