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Examination of surface nucleation during the growth of long alkane crystals by molecular dynamics simulation ALEXANDER BOURQUE, GREGORY RUTLEDGE, Massachusetts Inst of Tech-MIT — Crystal growth from the melt of n-pentacontane (C50) was studied by molecular dynamics simulation using a validated united atom model. By quenching below the melting temperature of C50 (370 K), propagation of the crystal growth front into the C50 melt from a crystalline polyethylene surface was observed. By tracking the location of the midpoint in the orientational order parameter profile between the crystal and melt, crystal growth rates between 0.015-0.040 m/s were observed, for quench depths of 10 to 70 K below the melting point. In this work, surface nucleation is identified with the formation of 2D clusters of crystalline sites within layers parallel to the propagating growth front, by analogy to the formation of 3D clusters in primary, homogeneous nucleation. These surface nucleation events were tracked over several layers and numerous simulations, and a mean first passage time analysis was employed to estimate critical nucleus sizes, induction times and rates for surface nucleation. Based on new insights provided by the detailed molecular trajectories obtained from simulation, the classical theory proposed by Lauritzen and Hoffman is re-examined.

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