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Molecular Simulation of Flow-Enhanced Crystal Nucleation in Alkane Melts DAVID NICHOLSON, GREGORY RUTLEDGE, Massachusetts Inst of Tech-MIT — Under typical processing conditions, the crystallization of polymer materials occurs far from equilibrium. In particular, the application of a flow field is known to drastically accelerate the kinetics of crystallization, and in turn alter the morphology and properties of the resulting material. It remains a significant challenge to establish the processing-structure-property relationships associated with crystallization under flow. Non-equilibrium molecular dynamics simulation has proven to be a useful investigative tool for the study of the early stages of flow-induced crystallization, known as flow-enhanced nucleation. Using this technique, nucleation studies were performed under shear and uniaxial extension for monodisperse melts of short (C20) and long (C150) alkanes, as well as for bimodal mixtures composed of both short and long chains. Through the application of a mean first-passage time-based analysis method, the effect of flow on the nucleation kinetics was quantified and classified in terms of an increase in the driving force for crystallization, reflected in the reduction of the free energy barrier, as well as a diffusive enhancement, reflected in the increase of the monomer attachment pre-factor. In bimodal blends with C150 fractions of 3-9 wt% chains, a drastic acceleration in the nucleation kinetics relative to monodisperse C20 was observed for strain rates intermediate to the inverse Rouse times of C20 and C150. For this range of strain rates, the long chains were found to preferentially participate in the formation of small clusters, and therefore serve as templates for the crystallization of the short chain fraction.

David Nicholson
Massachusetts Inst of Tech-MIT

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