Abstract Submitted
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Rotator phases and nucleation in polyethylene SCOTT MILNER, Penn State University — Experimental evidence has accumulated that polymer crystals often nucleate via a metastable, partially ordered "rotator" phase. To investigate this idea theoretically, we must calculate the bulk and interfacial free energies of the critical nucleus. We use our recent theory of the crystal-melt interface, which represents the amorphous region as a grafted brush of loops in a self-consistent pressure field, combined with estimates of bulk free energy differences based on experimental data, to calculate nucleation barriers and rates via rotator versus crystal nuclei for polyethylene. We find rotator-phase nucleation is indeed favored throughout the temperature range where nucleation is observed. Our methods can be extended to other polymers.

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