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A simple model for heterogeneous nucleation of isotactic polypropylene MICHAEL HOWARD, SCOTT MILNER, Penn State University — Flow-induced crystallization (FIC) is of interest because of its relevance to processes such as injection molding. It has been suggested that flow increases the homogeneous nucleation rate by reducing the melt state entropy. However, commercial polypropylene (iPP) exhibits quiescent nucleation rates that are much too high to be consistent with homogeneous nucleation in carefully purified samples. This suggests that heterogeneous nucleation is dominant for typical samples used in FIC experiments. We describe a simple model for heterogeneous nucleation of iPP, in terms of a cylindrical nucleus on a flat surface with the critical size and barrier set by the contact angle. Analysis of quiescent crystallization data with this model gives reasonable values for the contact angle. We have also employed atomistic simulations of iPP crystals to determine surface energies with vacuum and with Hamaker-matched substrates, and find values consistent with the contact angles inferred from heterogeneous nucleation experiments. In future work, these results combined with calculations from melt rheology of entropy reduction due to flow can be used to estimate the heterogeneous nucleation barrier reduction due to flow, and hence the increase in nucleation rate due to FIC for commecial iPP.

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