

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Influence of Stereotacticity Defects on the crystallization of Isotactic Polypropylene¹ XIAOFENG CHEN, RAHMI OZISIK, Rensselaer Polytechnic Institute, SANAT K. KUMAR, Columbia University, PHILLIP CHOI, University of Alberta, WAYNE L. MATTICE, University of Akron — Monte Carlo simulations of coarse-grained polypropylene on a high coordination lattice were performed to investigate the “equilibrium” crystallization behavior of isotactic polypropylene with and without stereotacticity defects at various concentrations and distributions. The formation of the helical structure, which forms the basic crystalline unit for isotactic polypropylene, is the focus of the current study. Results indicate that the effect of stereo defects is local - limited to two nearest neighboring repeat units on each side of the stereo defect. In addition, the influence of many stereo defects on the formation of helices is the sum of the influences of each individual stereo defect. The presence of stereo defects retards the crystallization temperature compared to isotactic polypropylene with no defects. This is expected as higher undercooling is necessary to form helices with imperfections.

¹The authors would like to thank National Science Foundation, Procter & Gamble Co., and Rensselaer Polytechnic Institute for financial support of this research.

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Date submitted: 04 Dec 2006

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