

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**The Influence of Stereoerrors on the Crystallization of Isotactic Polypropylene**<sup>1</sup> XIAOFENG CHEN, SANAT K. KUMAR, Chemical and Biological Engineering, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Crystallization behavior of four isotactic polypropylenes (iPP) with stereoerrors was studied by Monte Carlo simulation. All systems were equilibrated above the melting temperature ( $T_m$ ) and then cooled systematically to temperatures below the  $T_m$ . The conformations of the iPP chains were analyzed to characterize the crystallinity development in each system. The probability of helix formation, the average length of helices, and the fraction of repeat units involved in helical structures all increased as temperature decreased. As expected, the stereoregular iPP had the longest helical structures and the highest overall crystallinity compared to the other systems with stereoerrors. The overall crystallinity decreased with increasing number of stereoerrors. The influence of stereoerrors on the ability of iPP repeat units participation in helical structures was also investigated. The results showed that the stereoerrors can exist in helices but they strongly influence the ability of their neighbors to exist in helices.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant 0310596.

Rahmi Ozisik  
Rensselaer Polytechnic Institute

Date submitted: 22 Nov 2005

Electronic form version 1.4