

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Phase Transition Behavior of Isotactic Polypropylene Crystallized from a Homogeneous Melt**<sup>1</sup> XIAOFENG CHEN, SANAT K. KUMAR, Chemical and Biological Engineering, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — The equilibrium melting behavior of helical structures in isotactic polypropylene (iPP) was studied by a Monte Carlo simulation. It was found that the melting of iPP helical structure was an exponential process at high temperatures ( $T > 470$  K), whereas it becomes highly stretched at low temperatures ( $T < 400$  K). An estimate of the melting temperature was obtained from a novel application of the second moment of the waiting time distribution for helix melting as described by Odagaki (T. Odagaki, *Phys. Rev. Lett.* **1995**, 75, 3701). The calculated melting temperature was approximately 455 K, which is in surprisingly good agreement with experimental values. A second transition temperature was also observed at a lower temperature ( $T \sim 390$  K), which we can not explain by equilibrium considerations. We suggest that at this temperature, once a helix forms, it does not melt within the time scale studied.

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

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Date submitted: 22 Nov 2005

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