Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Molecular Simulation of the intercrystalline region in isotactic polypropylene VIKRAM KUPPA, GREGORY C. RUTLEDGE, Massachusetts Institute of Technology — Monte Carlo (MC) computer simulations are used to study the crystal-amorphous interlamellar phase in semi-crystalline isotactic polypropylene. This represents the first such study of the detailed atomic level structure of the interlamellar phase for a polymer with side groups. The polymer is modeled using a united atom force-field model. Replica exchange in energy space is required in addition to local conformation and topology altering MC moves to achieve effective sampling of phase space. The simulations reveal the temperature dependence of structural features such as mass and energy density profiles as well as population distributions of tails, loops and bridges associated with the fold surface. These results for polypropylene are compared and contrasted with previous results for the prototypical linear polymer, polyethylene, in order to study the effect of architectural complexity on structure and properties of semi-crystalline polymers

Vikram Kuppa
Massachusetts Institute of Technology

Date submitted: 24 Nov 2005 Electronic form version 1.4