

Abstract Submitted
for the OSS11 Meeting of
The American Physical Society

Effect of chain stiffness on structural and thermodynamic properties of polymers KIRAN KHANAL, JUTTA LUETTNER-STRATHMANN, University of Akron — The stiffness of the chains affects many properties of polymers. We investigate structural and thermodynamic properties of a bond-fluctuation lattice model for semiflexible polymer chains. Monte Carlo simulations for polymer melts for a range of values of the bending penalty, density, and temperature show elongation of the polymer conformations with increasing chain stiffness but no transition to a nematic phase. Results for average bead-bead interaction energy and bending energy were studied separately and showed that the bending energy is almost independent of the filling fraction, suggesting that the stiffness of the chains can be treated as a single chain property. We calculated the bending energy from the partition function of a pair of neighboring bonds and find excellent agreement between theory and simulation. Equation of state properties of the lattice model were determined from insertion methods and thermodynamic integration. We develop a theoretical description of these properties and use it to determine model parameters for real polymer melts from a comparison with experimental data.

Kiran Khanal
University of Akron

Date submitted: 10 Mar 2011

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