Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Monte Carlo simulations to study the effect of static and dynamic properties of polymer melts KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, Department of Physics, The University of Akron, Akron, Ohio — Static and dynamic properties of polymers are affected by the stiffness of the chains. In this work, we investigate structural and thermodynamic properties of a lattice model for semiflexible polymer chains. The model is an extension of Shaffer's bond-fluctuation model and includes attractive interactions between monomers and an adjustable bending penalty that determines the Kuhn segment length. This allows us to model melts of flexible and semiflexible chains. For this work, we performed Monte Carlo simulations for polymer melts with a range of bending parameters and densities. Results for chain dimensions show that the Kuhn segment length increases monotonously with the bending penalty and has a linear dependence for a range of bending parameters. Results for self diffusion constants show that the translational mobility is strongly reduced by increasing chain stiffness. We also investigate the effect of chain stiffness on thermodynamic properties of the melts.

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Date submitted: 07 Dec 2008 Electronic form version 1.4