Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Effect of pressure on orientational order in fluids of semiflexible polymer chains A Monte Carlo simulation study KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, Departments of Chemistry and Physics, University of Akron — Semiflexible polymer chains in solution show orientational order at sufficiently high concentrations and low temperatures. In melts of semiflexible chains, we expect packing effects to lead to an increase in orientational order with increasing pressure. In this work, we investigate this effect with Monte Carlo simulations 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, semiflexible, and rodlike chains. For this work, we performed Monte Carlo simulations for polymer melts with a range of bending parameters and densities. We determined the pressure in the athermal limit from chain and bead-insertion methods and use thermodynamic integration to obtain the equation of state at finite temperatures. We measure the orientational order parameter to describe long-range order in the system and we also determine local packing of chain segments.

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Date submitted: 29 Dec 2009 Electronic form version 1.4