Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

**Connections between static and dynamic properties of athermal polymer melts: a Monte Carlo simulation study** NENAD STOJILOVIC, Physics Department, John Carroll University, JUTTA LUETTMER-STRATHMANN, Departments of Physics and Chemistry, The University of Akron — The motion of individual chains in polymer melts and blends is governed by local friction and entanglement effects. In simulations and experiments it can be difficult to separate these effects since both local friction coefficients and entanglement lengths depend on the thermodynamic state and the chain structure and since many systems display neither ideal Rouse nor fully entangled dynamics. In this work, we investigate local and chain dynamics of athermal polymer melts with Monte Carlo simulations of two versions of Shaffer's bond- fluctuation model [J. S. Shaffer, J. Chem. Phys. 101, 4205 (1994)]. In the first version, bonds are allowed to cross each other with the result that the chains do not entangle; in the second, bond crossings are prohibited and entanglement effects become apparent. Since both versions of the model have very similar static properties, local friction and entanglement effects can be separated. With simulations for a range of densities and chain lengths, we investigate connections between static and dynamic properties, in particular, scaling with the packing length and the size of the moving segment responsible for local friction.

Nenad Stojilovic
Physics Department, John Carroll University, University Heights, OH 44118

Date submitted: 13 Dec 2007 Electronic form version 1.4