Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Highly constrained polymer dynamics with an enhanced bond-fluctuation model[1] FRANK BENTREM[2], COLIN MCFAUL, Department of Physics and Engineering Physics, Tulane University, New Orleans, Louisiana 70118, USA — We introduce a generalization to the bond-fluctuation model for simulating polymer dynamics in a highly constrained environment. The technique is applied to the quenching of self-attracting polymer chains which demonstrates a three-fold collapse. Both the extent and dynamics of the collapse are greatly enhanced by using the generalized bond-fluctuation model where the bond length $l = \sqrt{8}$ (in units of the lattice spacing) is explicitly utilized. We also show that lattice effects in dense melts ($\phi > 0.5$) are alleviated with this enhancement. Efficiency is maintained by implementing a simple check to prevent phantom chain dynamics.

[1]Sponsored by the Office of Naval Research through the Naval Research Laboratory's Advanced Graduate Research Program.
[2]Present address: Marine Geosciences Division, Naval Research Laboratory, Stennis Space Center, Mississippi 39529, USA

Frank Bentrem
Department of Physics and Engineering Physics,
Tulane University, New Orleans, Louisiana 70118, USA

Date submitted: 09 Dec 2009 Electronic form version 1.4