Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Coarse graining of atactic polystyrene and its derivatives[1]
ANUPRIYA AGRAWAL, DVORA PERAHIA, Clemson University, GARY S. GREST, Sandia National Laboratories — Capturing large length scales in polymers and soft matter while retaining atomistic properties is imperative to computational studies of dynamic systems. Here we present a new methodology developing coarse-grain model based on atomistic simulation of atactic polystyrene (PS). Similar to previous work by Fritz et al., each monomer is described by two coarse grained beads. In contrast to this earlier work where intramolecular potentials were based on Monte Carlo simulation of both isotactic and syndiotactic single PS molecule to capture stereochemistry, we obtained intramolecular interactions from a single molecular dynamics simulation of an all-atom atactic PS melts. The non-bonded interactions are obtained using the iterative Boltzmann inversion (IBI) scheme. This methodology has been extended to coarse graining of poly-(t-butyl-styrene) (PtBS). An additional coarse-grained bead is used to describe the t-butyl group. Similar to the process for PS, the intramolecular interactions are obtained from a single all atom atactic melt simulation. Starting from the non-bonded interactions for PS, we show that the IBI method for the non-bonded interactions of PtBS converges relatively fast. A generalized scheme for substituted PS is currently in development.

[1]We would like to acknowledge Prof. Kurt Kremer for helpful discussions during this work.

Anupriya Agrawal
Clemson University

Date submitted: 15 Nov 2013 Electronic form version 1.4