Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Properties of Coarse-Grained Polymer Models: Statics, Dynamics, and Crystallinity[1] GARY GREST, K. MICHAEL SALERNO, Sandia National Laboratories, ANUPRIYA AGRAWAL, DVORA PERAHIA, Clemson University — To capture large length and time scales, coarse-grained (CG) models that combine multiple atoms into one bead have been developed to model polymer melts. In the process microscopic detail is discarded in exchange for computational efficiency. However it is not well-understood how the scale of coarse-graining affects the polymer structure and dynamics. We compare results of atomistic simulations with CG models in which each CG bead represents three, four, or six methylene groups for $C_{96}H_{194}$, $C_{480}H_{962}$, and $C_{960}H_{1922}$. The CG potential is developed at 500K by iterative Boltzmann inversion. While static properties such as end-to-end distance and radius of gyration are captured by all CG models, the entanglement length deviates from experimental results with increased CG scale. The mean squared displacement of CG models is used to determine scale factors between the atomistic and CG models. During cooling to low temperature, the three and four-carbon models form a semi-crystalline structure while the six-carbon model and a four-carbon model based on the MARTINI force field remain amorphous at all temperatures. These findings show that the level of coarse-graining and CG interactions can strongly affect model temperature transferability.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's NNSA under contract DE-AC04-94AL85000.

K. Michael Salerno
Sandia National Laboratories

Date submitted: 14 Nov 2014 Electronic form version 1.4