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**Dynamics in entangled polyethylene melts using coarse-grained models** BRANDON L. PETERS, GARY S. GREEST, Sandia National Laboratories, K. MICHAEL SALERNO, U. S. Naval Research, ANUPRIYA AGRAWAL, Washington University in St. Louis, DVORA PERAHIA, Clemson University — Polymer dynamics creates distinctive viscoelastic behavior as a result of a coupled interplay of motion on multiple length scales. Capturing the broad time and length scales of polymeric motion however, remains a challenge. Using polyethylene (PE) as a model system, we probe the effects of the degree of coarse graining on polymer dynamics. Coarse-grained (CG) potentials are derived using iterative Boltzmann inversion (iBi) with 2-6 methyl groups per CG bead from all fully atomistic melt simulations for short chains. While the iBi methods produces non-bonded potentials which give excellent agreement for the atomistic and CG pair correlation functions, the pressure  $P = 100\text{-}500\text{MPa}$  for the CG model. Correcting for potential so  $P = 0$  leads to non-bonded models with slightly smaller effective diameter and much deeper minimum. However, both the pressure and non-pressure corrected CG models give similar results for mean squared displacement (MSD) and the stress auto correlation function  $G(t)$  for PE melts above the melting point. The time rescaling factor between CG and atomistic models is found to be nearly the same for both CG models. Transferability of potential for different temperatures was tested by comparing the MSD and  $G(t)$  for potentials generated at different temperatures.

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