

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Coarse-Grained Simulations of PEO/PMMA Blends PRAVEEN DEPA, CHUNXIA CHEN, JANNA MARANAS, Pennsylvania State University — Coarse-graining involves mapping successive atoms along a polymer chain to larger coarse-grained beads, which are then simulated using conventional molecular dynamics techniques. The interaction between the coarse-grained [CG] beads is parameterized so as to reproduce static properties observed in the underlying atomistic simulations. We extend this methodology to blends by developing CG models for poly(ethylene oxide) [PEO], poly(methylmethacrylate) (PMMA) and PEO/PMMA blends. In the case of PEO, six united atoms were mapped to a CG bead with the center at every other oxygen atom and for PMMA, each monomer was replaced with two CG beads, one centered along the main chain and the other centered at the ester-oxygen on the side group. The CG models reproduce static properties for both components. Dynamic properties evolve correctly if rescaled by a constant factor, specific to each component. The CG model is then used to simulate larger system for longer times such that whole chain dynamics can be accessed and compared to local dynamics.

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Date submitted: 04 Dec 2005

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