Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Coarse-graining and Multiscale Modeling of Polymeric Materials IVAN LYUBIMOV, MARINA GUENZA, University of Oregon — Dynamics of macromolecules are characterized by the presence of several length scales in which relevant phenomena take place. Theoretical models play a pivotal role in building the infrastructure that allows one to model multiscale properties. Starting from the Ornstein- Zernike equation we derive analytical methods that coarse-grain the structure of polymeric liquids (homopolymer melts, diblock copolymers, and polymer mixtures) at different length scales of interest. These methods provide effective potentials input to mesoscale simulations. Information obtained from simulations, performed at the united-atom and at the coarse-grained scales, is combined in an original multiscale modeling procedure, resulting in the complete physical picture of the system across the many length scales of interest.

Marina Guenza
University of Oregon

Date submitted: 14 Jan 2008 Electronic form version 1.4