

## **224f Peo/Pmma Blend: a Coarse-Grained Approach to Observe Entangled Dynamics**

*Praveen K. Depa and Janna K. Maranas*

Coarse-grained force fields have been developed for extending length and time scales in polymer simulations. In coarse-graining, successive atoms along the chain are mapped on to larger coarse-grained beads, which are then simulated using conventional molecular dynamics techniques. We present a procedure to develop a coarse-grained model for PEO/PMMA blends at different compositions and temperatures. The coarse-grained force field is parameterized so as to reproduce structural features observed in the underlying atomistic simulations of the blend. This coarse-grained force field is then used to simulate larger chain lengths for longer times, allowing us to observe entangled dynamics. The dynamic properties from coarse-grained molecular dynamics simulations are then compared with experiments that measure long time relaxations of the chain.