Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Mesoscale simulation of entangled polymers: Part I. Coarse-Grained level Tunable DPD JOAO MAIA, SHAGAHYEGH KHANI, MIKIO YAMANOI, Case Western Reserve University — Dissipative Particle Dynamics (DPD) is a coarse-grained molecular dynamics based simulation method that has shown a very good potential in computational modeling of soft matter. However, it is associated with deficiencies in simulating the dynamics of entangled polymer systems. For instance, due to the upper limit of coarse-graining level the method could not be applicable to the whole mesoscopic range. Therefore, our group has proposed a new concept of DPD named Coarse-Grained level tunable DPD method in which the level of coarse graining can be tuned by adjusting the simulation parameters considering an energy balance in the system. The unphysical bond crossings that are artifacts of the soft potentials are prevented by applying an entanglement potential between the bonds. The performance of the method in capturing the entanglement effect is investigated by calculating the static and dynamic properties of polymers in entangled state. Linear and non-linear viscoelastic properties can also be predicted by the CG level tunable DPD method reasonably well. Moreover, this method is able to reproduce the 1.0 to 3.4 transition in power index of the zero shear viscosity with molecular weight which captures the Rouse to reptation behavior in entangled polymer systems.

Shaghayegh Khani
Case Western Reserve University

Date submitted: 15 Nov 2013 Electronic form version 1.4