Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Hierarchical assembly of block copolymer micelles into reversible networks: MC simulations ZILU WANG, Physics Department and Institute of Materials Science, University of Connecticut, ELENA DORMIDONTOVA, Institute of Materials Science, University of Connecticut — The rapid development of nanoscience has considerably expanded the range of building blocks for complex self-assembled nanostructure formation, which show great potential for numerous advanced applications. We apply Monte Carlo simulations to gain understanding of molecular mechanism of self-assembly of nanostructures formed by diblock copolymer micelles interconnected by means of metal-ligand complexation. These systems exhibit interesting chemical and mechanical stimuli-responsive behavior and possess two levels of self-assembly: 1) self-assembly of diblock copolymers into micelles and 2) reversible inter-micelle bridging by coordination bonding between metal ions and ligands attached to the corona of nanoparticles, which is responsible for the network viscoelastic properties. Using MC simulations we investigate the effect of metal-ligand complexation on diblock-copolymer micelle formation and vice versa. We analyze the extent of intra- and inter-micelle loops and bridges formed by metal-ligand complexation in relation to the degree of crosslinking and elastic properties of the network. The effect of polymer concentration, hydrophilic block length, metal to oligomer ratio and type of complexation (2:1 or 3:1) on equilibrium properties of reversible networks will be discussed.

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Date submitted: 14 Nov 2014 Electronic form version 1.4