Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

A theoretical study of polymer grafted nanoparticles as fillers in polymer nanocomposites ARTHI JAYARAMAN, University of Colorado-Boulder, KENNETH SCHWEIZER, University of Illinois-Urbana — We have generalized the microscopic Polymer Reference Interaction Site Model (PRISM) theory to study the structure and phase behavior of polymer-tethered spherical nanoparticles (fillers) in a homopolymer matrix. In the absence of a polymer matrix, melts of polymer-tethered nanoparticles show strong concentration fluctuations indicative of aggregate formation and/or a tendency for microphase separation as the total packing fraction and/or nanoparticle attraction strength increase. In the presence of a polymer matrix there is competition between nanoparticle attractions, steric repulsion between grafted polymers, and polymer matrix induced depletion-like attraction. For single tethered particles, volume of the tether being equal to the volume of the nanoparticle, the apparent microphase spinodal curve exhibits both dilution-like and depletion-like features, and a non-monotonic dependence on matrix chain length. As the particle size and tether length are increased, such that the total space filling volume of the tether continues to equal the nanoparticle volume, the shape of the microphase spinodal curve remains unchanged, but the effect of matrix polymer chain length on the spinodal temperature diminishes. The effect of various parameters on the spinodal temperature will be presented.

Arthi Jayaraman
University of Colorado-Boulder

Date submitted: 29 Nov 2008 Electronic form version 1.4