Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

A coarse-grained molecular dynamics approach to shear-directed assembly of nanoparticle arrays in amphiphilic block copolymer solutions BRYAN ROLFE, Cornell University, JAEHUN CHUN, Pacific Northwest National Laboratory, YONG JOO, Cornell University, ENERGY AND ENVIRONMENT DIRECTORY PACIFIC NORTHWEST NATIONAL LABORATORY COLLABORATION — Experiments by Pozzo and Walker (2007) demonstrated shear ordering of binary nanoparticle block copolymer micelle crystals and its potential in the development of new nanostructured materials. Specifically, they have shown that nanoparticles occupying interstitial sites within the micelle crystal affect a low-shear, long-range order and that the shear type and rate are important to the crystal structure. However, the connection between macroscopic variables and resulting crystal structure is yet to be understood. We present results which elucidate the underlying mechanisms governing shear-directed assembly of these binary nanocrystals. Our approach employs a coarse-grained molecular dynamics model (CGMD) that includes the hydrodynamics of the solvent and preserves dynamic effects by making no assumptions regarding the micelle structure. In fact, micelle self-assembly of the amphiphilic block copolymers occurs in-situ with the nanoparticles along with the shear ordering of the binary crystal. Tunability of the crystal structure is determined by varying shear rates/types, nanoparticle size/concentration, and block copolymer chemistry as simulation parameters. The simulation predicted results of shear-directed assembly of nanoparticles will be compared to the experimental results.

Bryan Rolfe
Cornell University

Date submitted: 11 Nov 2011 Electronic form version 1.4