MODELING AND SIMULATION OF SOFT-PARTICLE COLLOIDAL SYSTEMS UNDER DYNAMIC ENVIRONMENTAL GRADIENTS

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Controlled assembly in soft-particle colloidal suspensions is a technology poised to advance manufacturing methods for nano-scale templating, coating, and bio-conjugate devices. Applications for soft-particle colloids include photovoltaics, nanoelectronics, functionalized thin-film coatings, and a wide range of bio- conjugate devices such as sensors, assays, and bio-fuel cells. This presentation covers the topics of modeling and simulation of soft-particle colloidal systems over dewetting, evaporation, and irradiation gradients, including deposition of particles to surfaces. By tuning particle/solvent and environmental parameters, we transition from the regime of self-assembly to that of controlled assembly, and enable finer resolution of features at both the nano-scale and meso-scale.

We report models of interparticle potentials and order parametrization techniques including results from simulations of colloids utilizing soft-particle field potentials. Using LAMMPS (Large-Scale Atomic/Molecular Massively Parallel Simulator), we demonstrate effects of volume fraction, shear and drag profiles, adsorbed and bulk polymer parameters, solvent chi parameter, and deposition profiles. Results are compared to theoretical models and correlation to TEM images from soft-particle irradiation experiments.