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Self-Assembly of Diblock Copolymers/Au Nanoparticle Nanocomposites in Thin Films

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Polymer nanocomposites have been shown to exhibit unique behavior in permeability, catalytic activity, and optical and magnetic properties. In many cases, the ability to exploit nanoparticle properties for potential applications requires highly ordered arrays of nanoparticles in matrices [1-3]. Intense research has been underway for the development of well-controlled particles in a copolymer matrix by tailoring nanoparticles with homopolymers as a surfactant [4-7]. Traditional methods to form nanocomposites typically do not result in predictable material properties because of particle agglomeration that leads to architectural inhomogeneities. To have well-controlled behavior of these novel nanocomposites, a detailed understanding of the morphology during processing is important to achieve the desired engineering goal. In this study, we developed a novel technique to synthesize polystyrene-*b*-poly(2-vinylpyridine) (PS-PVP) nanocomposites with ordered arrays of gold nanoparticles and observed the structure of composites using transmission electron microscopy (TEM).

Bulk and thin films of the nanocomposites were investigated in order to understand the effects of copolymer molecular weight, volume fractions of the polymers, size and concentration of the functionalized nanoparticles, thin film vs. bulk architecture and annealing with solvent and temperature on the phase behavior and structural order in the composites. In addition to TEM we applied appropriate methodologies to use small angle X-ray scattering (SAXS) at the Argonne National Laboratory Advanced Photo Source (APS) to probe the nanostructure in thin films and bulk and their formation with *in situ* studies.

It was observed that the addition of nanoparticles swelled the preferred domain causing a phase transformation to occur. We have generated phase diagrams as a function of the relative length of diblocks (*f*) and the concentration of nanoparticles. Morphologies as lamellar structure, hexagonally packed cylinder, and centered-cubic packed spheres were obtained. The overall goal of this research is to study how the molecular properties of polymers as well as nanoparticles affect the controlled ordering of nanoparticles in polymer matrices. With a systematic study we aim to develop a fundamental understanding of molecular ordering mechanism(s) that will result in predictable characteristics of the synthesized nanocomposites.

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