MRSEC SEMINAR SERIES

"Thermodynamic and kinetic routes for the design of polymer nanocomposites."

Polymer nanocomposites have the potential for a wide array of applications, ranging from light-weighting structural materials, to conductive polymer films, to metamaterials with exotic optical properties such as cloaking. In applications involving polymer nanocomposites, controlling the dispersion and assembly of the nanoparticles is one of the most critical aspects of their design, and the final distribution of nanoparticles is a complex interplay of both processing conditions and the entropic and energetic interactions between the matrix polymers, nanoparticles, and any surface functionalization on the particles. As a result, it is often challenging for experimentalists to anticipate the final structure of a polymer nanocomposites. Historically, various theories have played a significant role in developing our understanding of polymeric materials, but many require significant approximations to study composites or are challenged by inhomogeneous (phase separated) structures. In this talk I will briefly describe our work that extends polymer field theory to polymer nanocomposites and other materials where correlation effects become important, such as polymer nanocomposites, and I will discuss its application in two example systems. First, we have developed strategies for achieving vertically-oriented nanorods in block copolymer thin films for use as thermally conductive membranes, which has recently been borne out in experiments. We find that the block copolymer films must be carefully designed to prevent segregation of nanoparticles to defects, and processing can play a large role in the final distribution of the nanoparticles. Second, I will show recent results on how we can employ evolutionary design strategies to tune the chemistry of polymer-grafted nanoparticles so that they self-assemble into targeted structures. We find that the stability of the resulting structure against fluctuations in both the surface chemistry and the nanoparticle concentration depends on the targeted structure.

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