Polymer-Inorganic Nanocomposites: Theoretical Studies of Thermodynamics and Phase Behavior

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Abstract

Polymer nanocomposites (PNC) represent a new class of materials that is being actively developed for a wide variety of commercial applications (automotive, packaging, cosmetics, electronics, etc.) Particular attention is paid to three main classes: (i) polymer/metal nanoparticle composites; (ii) polymer/carbon nanotube composites; (iii) polymer/clay nanocomposites. Significant successes have been achieved in making these systems yet our understanding of their behavior is still rather limited.

In my talk, I will describe recent theoretical efforts aimed at the understanding of thermodynamics and phase behavior of PNC’s. In particular, we will examine theoretical models describing (i) self-assembly of block copolymer/metal nanoparticle mixtures, and (ii) morphology of clay platelets in homogeneous polymer melts. We will see that the size and geometry of the nanoscale fillers play a crucial role in determining the morphology and phase behavior of the nanocomposite. It is shown that for the case of small (5—10 nm) nanoparticles, self-assembly can indeed guide the system towards thermodynamically stable morphologies (e.g., lamellar morphologies with particles segregated into one block or at the interfaces between lamellar domains). In the case of clays, on the other hand, thermodynamically advantaged morphology is often the “macrophase separated” state where clay platelets are segregated from the matrix; it becomes necessary, therefore, to be able to preserve the system in a non-equilibrium state (which is often difficult to do). Overall, theoretical predictions - while imperfect - could serve as good guidelines for the composite formulation design.

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