4bh Morphology and Structure in Polymer Nanocomposites and Compound Droplets

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The ability to control structure at the nano- to micro-scale is of great importance in the design of new materials for any number of applications. I present research in two areas motivated by this fact.

1.Aggregation and self-assembly in polymer nanocomposites.

Using molecular dynamics (MD) simulations I investigate the properties of polymer melts containing particles of sizes comparable to chain length. The addition of such particles is well known to enhance the mechanical properties of polymer materials. I will discuss the effective interaction of particles mediated by a polymer matrix with particular attention to the ability to modify these interactions by varying particle shape. A promising application is the use of nanocomposite coatings to repair solid surfaces. I will show that depletion forces drive particles towards the surface and that this phenomenon can be used to "heal" nanoscale cracks and scratches which are difficult to detect. I will also discuss the behavior of the melt near a surface [1].

2.Compound droplets in polymer blends

Multicomponent systems of three or more phases, where the dispersed phase is itself a discrete polymer blend, enhance our capacity to design new materials. I have previously [2] examined hydrodynamic phenomena in these systems. I will also discuss current work on the effect of the molecular weight dependent curvature contribution to the free energy of polymer blends [3]. I will show how this term can lead to morphologies and dynamical behavior for compound droplets different than those predicted by interfacial tension alone.

[1] K. A. Smith, M. Vladkov and J. L. Barrat, "Polymer melt near a solid surface: A molecular dynamics study of chain conformations and desorption dynamics", Macromol., 38, 571, (2005).

[2] K. A. Smith, J. M. Ottino and M. Olvera de la Cruz, "Encapsulated drop breakup in shear flow", Phys. Rev. Lett., 93, 204501, (2004) ; K. A. Smith, F. J. Solis, L. Tao, K. Thornton and M. Olvera de la Cruz, "Domain growth in ternary fluids: A level set approach", Phys. Rev. Lett., 84, 91, (2000).

[3] H. Tang and K. F. Freed, "Free energy functional expansion for inhomogeneous polymer blends", J. Chem. Phys., 94, 1572 (1991).