Distinguished Lecture Series

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Modeling the Behavior of Stimuli-Responsive Polymeric Materials

Microcapsules that release encased nanoparticles and self-oscillating gels that display novel periodicity have been studied using a variety of coarse-grained computational models. The nanoparticles are treated as “tracer particles” and their motion is modeled via a Brownian dynamics simulation. An imposed pressure gradient drives the microcapsules along an adhesive substrate and the particles are released from the surface of this mobile capsule. We determine how the elasticity of the capsule, the strength of the capsule–surface adhesion and the diffusion coefficient of the nanoparticles affect how the particles are adsorbed onto a surface. The findings yield guidelines for optimizing the efficiency of microcapsule carriers in the targeted delivery of nanoparticles and provide guidelines for creating “repair and go” microcapsules that can monitor and repair damage in surfaces.

In the second study, we develop an efficient model for responsive gels that captures large-scale, two-dimensional deformations and chemical reactions within a swollen polymer network. In gels undergoing the oscillatory Belousov-Zhabotinsky reaction, we observe traveling waves of local swelling that give rise to distinctive oscillations in the gel’s shape. The observed patterns depend critically on the gel’s dimensions. The approach provides a useful computational tool for probing the dynamics of chemo-mechanical processes and uncovering morphological transformations in responsive gels.

Thursday, January 25, 2007
11 AM, Building 224, Room B-245

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