Center for Molecular and Engineering Thermodynamics

CMET Seminar

- **December 20, 2007**
- **11:00 A.M.** (refreshments available at 10:45 A.M.)
- **366 Colburn Laboratory**

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"Orientation Distribution and Transitions in Polymer-Dispersed Liquid Crystalline Materials"

Orientation distributions in droplets of liquid crystals with homeotropic anchoring are computed with a simulated annealing algorithm that minimizes the free energy of the Oseen-Frank continuum theory algorithm [Goyal and Denn, Phys. Rev. E, 75, 021704 (2007)]. The droplets exhibit multiple orientational steady states that are separated by finite energy barriers over the entire range of the dimensionless ratio of surface to elastic forces, with maximum transition energy densities of the order of 2,000 J/m^3 (Pa) for a typical liquid crystalline droplet with a spherical radius of 1 μm. We also compute the surface-induced droplet morphology and the free energy pathway as a cylindrical nematic liquid crystalline filament passes through a sequence of sinusoidal perturbations and breaks up into droplets. A first-order morphological transition with a finite energy barrier is required when the perturbation amplitude exceeds a critical value. This result is consistent with a kinetic trapping explanation proposed by Inn and Denn [J. Rheology, 49, 887-895 (2005)] for a delayed transition from a gel to a dispersed droplet morphology in blends of 4'-octyl-4-biphenylcarbonitrile (8CB) and poly(dimethyl siloxane).

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