

259f Structure Development in Phase-Separating Complex Fluid Systems

David M. Hall, Turab Lookman, and Sanjoy Banerjee

Advances in synthetic methods for producing block and graft copolymers have enabled the construction of new multiphase complex fluid formulations in which the domain size falls in the nanometer range and the geometrical arrangement of the domains can be precisely controlled by varying copolymer architecture and composition variables. The influence of processing flows on the bulk properties of such formulations is an important consideration for a variety of industries, such as paints, adhesives, coatings, polymer alloys, personal care products, cosmetics, and processed foods. Because the experimental design space for these materials is vast, theoretical and computational methods are of increasing interest as tools to be utilized in the design process.

A technique for simulating complex fluids in systems out of equilibrium is discussed. It is a generalization of two powerful mesoscale methods, self-consistent field theory, and the two-fluid model for viscoelastic hydrodynamics. This approach is shown to capture both the complex self-assembly and phase-separation found in multi-block copolymer systems, as well as the effects associated with flows, including those due to viscoelasticity.