

“Directed Assembly at the Nanoscale, and its Application to Nanoscale Fabrication”

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There is considerable interest in devising nanofabrication strategies that rely on the molecular self-assembly of complex fluids and materials. Our efforts over the past several years have been focused on devising strategies to drive and direct that self assembly, largely by developing multiscale modeling models and methods capable of predicting the structure and properties of complex fluids and materials under external fields, including confinement, electric fields, or flow fields. These models and methods can vary considerably in nature and level of resolution, depending on the system and issues of interest.

In this presentation I will provide an overview of various modeling approaches, along with their usefulness and limitations, in the context of two distinct nanofabrication platforms of current interest. The first is concerned with the formation of ordered, defect-free block copolymer structures on nanopatterned substrates. A new mesoscopic formalism has been developed to describe the structure and dynamics of block copolymer blends and composites, and we use it to explain the effects of surfaces and different types of confining walls on the free energy (and the concomitant stability) of a variety of morphologies of interest for lithographic fabrication. Many of these morphologies represent non-equilibrium states that are accessed by specific processing routes, and simulations can be used to discern the boundaries between such states and stable, equilibrium morphologies. Some of the insights provided by our work have led to a number of applications that are currently being pursued by the semiconductor and data storage industries; a brief overview of some of those applications will be presented.

The second application is concerned with the development of liquid-crystal based biosensors. A multiscale model has been used to design liquid-crystal based devices for detection of biological molecules or toxins. In one implementation, nanoscale particles self-assemble into highly regular structures, including chains, upon exposure to specific chemicals. In a different implementation, liquid crystal nanodroplets are shown to adopt distinct configurations upon exposure to specific analytes. As discussed in this presentation, the models can be used to explain the defects and transmission images that arise in laboratory experiments. Theoretical calculations and simulations can then be used to identify metastable states that are particularly responsive to external perturbations, thereby offering a route for preparation of systems that offer an enhanced response to external stimuli. A recent application of such ideas will be discussed in which sensors for detection of extremely low levels of endotoxin have been demonstrated.