Modeling particle transport in lithographically directed, evaporation driven self-assembly systems

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Topographically directed, evaporation driven self-assembly (EDSA) of nanoparticles is a promising manufacturing technique that combines the control of top-down lithography with the speed of bottom-up self-assembly.[1,2] We have developed a modeling methodology, using computational fluid dynamics (CFD), for simulating the global regime of directed EDSA. The global regime considers the macro-scale distribution of the particles in the colloidal solution. The distribution is determined by the forces exerted on the particles due to the fluid motion, which is driven by evaporation and influenced by pinning of the contact line by lithographically defined surface features.[3]

We have simulated the evaporation-driven flows generated within a volume of fluid that is changing in size under various pinning conditions. The shape of the fluid volume is determined from free surface simulations using energy minimization techniques.[4] We have used this methodology to predict the evolution of the particle concentration distribution and to provide useful information about the time scales required to generate a sufficient concentration of nanoparticles near a pinning feature so that self-assembly will occur. The model is one part of a hierarchical set of multi-level engineering models that can be used to study the details of directed self-assembly processes.

The global model has been experimentally verified against the benchmark case of a self-pinning, colloidal droplet by measuring the intensity of fluorescent nanoparticles within the droplet as evaporation occurs (Fig 1). The strength of the model lies in its ability to simulate the evaporation of arbitrarily pinned droplets (Fig 2). During EDSA manufacturing processes, colloidal fluid is pinned by a series of features on the substrate. We have used the model to explore the effect of process parameters, such as evaporation rate, wetting characteristics, and pinning geometry, on the manufacturing capabilities of the technique.

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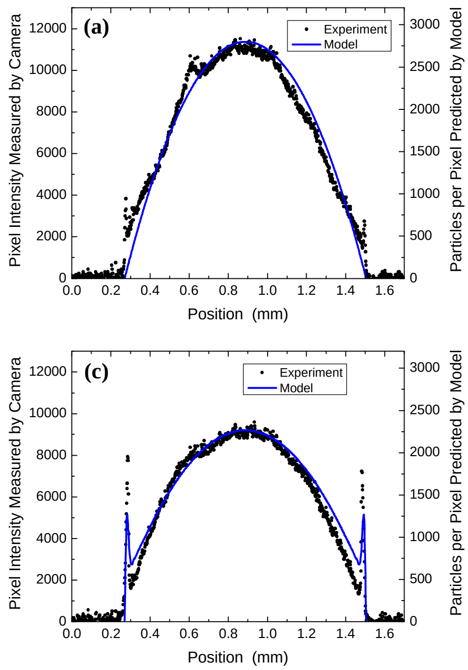

Figure 1. The measured intensity of fluorescing nanoparticles within a droplet is related to the distribution of particle concentration. The recorded intensity and predicted particle count along the diameter of a circular droplet during evaporation is shown at (a) 0 s, (b) 10 s, (c) 20 s, and (d) 30 s. The model accurately predicts the rate of particle transport to the pinned contact line, as well as the formation of a high concentration ring at the perimeter of the droplet.

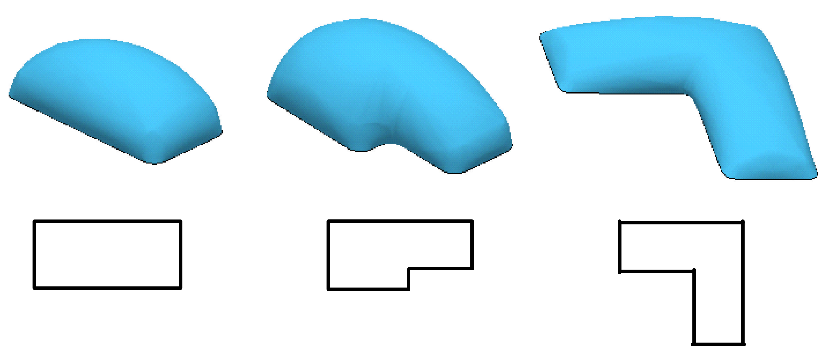

Figure 2. Several droplet shapes and associated lithographic patterns investigated through the coupling of surface energy minimization methods with CFD modeling.