Transient multiscale modeling of electrochemical deposition

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Abstract

We present results of transient multiscale simulations of electrochemical reactors, watching the time evolution of deposition on a feature scale. In order to perform these multiscale simulations we have coupled a reactor-scale mass and momentum transport simulator to a feature scale topography simulator. PHASTA[1], the reactor scale fluid flow simulator, tracks the convective diffusive transport of reactants to the surface of a patterned wafer. At the surface, EVOLVE[2], a feature scale topography simulator, takes over and uses the concentrations from PHASTA as boundary conditions at the top of the feature scale solution domain and uses the location of the feature on the wafer to retain the state of the feature between time steps. EVOLVE simulates the actual deposition process on the patterned surface through an iterative finite element solution of the concentration and potential fields. EVOLVE uses this information to determine the flux of reactants and by-products to and from the surface and feeds this information back to the reactor-scale simulation.

On the reactor scale, a locally refined mesh is used to maintain spatial resolution in regions in which fluid flow or concentration fields are changing quickly without requiring excessive calculations in regions of smaller gradients. We describe the state of the feature by a small number of variables which we track along the wafer surface over time. This allows us to indicate the current geometry of partially filled features anywhere on the wafer surface as a function of deposition time.

1. C. H. Whiting and K. E. Jansen, Intl. J. Num. Meth. Fluids, 35, p. 93 (2001). 2. EVOLVE is an extensible topography simulation framework. EVOLVE 5.0i was released in June 1999.