380a Multiscale Model for Plasma Enhanced Deposition on Nanostructures

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We present an integrated experimental/modeling investigation of a procedure to coat nanofibers using plasma enhanced physical vapor deposition. The interrelationships among processing factors for the transport and deposition are investigated here from a detailed modeling approach. Solution strategies that couple continuum and atomistic models are used. At the continuum scale, transport dynamics near the nanofiber are described. At the atomic level, molecular dynamics (MD) simulations are used to study the deposition and sputtering mechanisms at the coating surface. Ion kinetic energies and fluxes are passed from the continuum sheath model to the MD simulations. These simulations calculate sputtering and sticking probabilities that in turn are used to calculate parameters for the continuum transport model. The continuum transport model leads to the definition of an evolution equation for the coating free surface. This equation is solved using boundary perturbation and level set methods to determine the coating morphology as a function of operating conditions. Experimental and modeling results are compared.