# Multiscale Process Modeling in Microelectronics

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Abstract

We discuss and show examples of an approach to simulating grain structure development during deposition from the vapor phase, either by physical vapor deposition (PVD) or chemical vapor deposition (CVD). Using a grain continuum simulation software previously reported on, PLENTE, we perform simulations of deposition into developing grain structures in which re-emission and line-of-sight redistribution of unconsumed reactants is an important phenomenon. This simulation requires the repeated calculation of a "view factor matrix" of transmission probabilities that is obtained using direct sampling via ray traces. Direct sampling is also used to obtain the initial fluxes to the structure from the source gas, starting with structures encapsulated from atomistic simulations. EVOLVE is used to perform the kinetics and re-distribution of fluxes based on the local chemical reaction rates. We include crystallograpic information provided by PLENTE, in order to account for energetically preferable growth planes. The requireddiffusivities and orientation-dependent kinetics come from atomistic calculations.

It is observed that the density of the grain structure is significantly affected by the kinetics of the reaction relative to the amount of flux to the surface, and that faster reactions result in less redistribution of material, and higher void fractions in the developing grain structure. Also, faceting is observed due to the orientation effects incorporated through the kinetic expressions.