309c Development of Approximate Growth Models to Control Thin-Film Deposition Using Stochastic Differential Equations

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Thin film deposition is an important process in semiconductor manufacturing. Lately,considerable research effort is being directed towards development of optimization and control strategies based on detailed macroscopic and microscopic models. However, high computational requirements associated with these models have led to development of reduced, "computational friendly", process models [2, 3], to perform these tasks.

We focus on the development of computationally efficient dynamic process models for the evolution the microscopic properties during thin-film growth. Specifically, we derive a set of coupled stochastic differential equations (SDEs) for the temporal evolution of the dominant surface characteristics during the deposition process. These SDEs are an approximation of kMC-based detailed process descriptions and capture the dominant traits of the surface of the growing film. The motivation behind this approach is to develop a predictive microscopic optimization and control methodology based on reduced process models that circumvent the computational issues related to direct atomistic simulations such as kMC or MD. The variables that capture the dominant traits of the film surface can be categorized based on the nature of the information contained within them, i.e., statistical or spectral. The variables linked to statistical information describe the unavailable discrete lattice height distribution function and are obtained from Charlier Series B type expansion based on Poisson distribution. The variables linked to the spectral information describe the lateral correlation between lattice locations and are derived from a number of two-point correlation functions. The issue of uniqueness of surfaces having a given set of statistical and spectral parameters with respect to kMC simulations is also discussed, and we demonstrate that by incorporating a su±cient amount of statistical and spectral information through a finite (and small) number of parameters, the dominant growth dynamics can be adequately captured. For the identification of the state-space model, we employ Carlemann Linearization in conjunction with Maximum Likelihood Estimation [1] and derive a set of SDEs that govern the dynamic behavior of system. The proposed approach is employed towards the control of a conceptual deposition process which describes film growth under adsorption and surface diffusion with first neighbor interactions. A reduced SDE-based process model is constructed from the data obtained through kMC simulations of this deposition process under a wide range of macroscopic process conditions (e.g., wafer temperature and flux of reactants). Subsequently, the reduced process model is successfully employed as a basis for controller synthesis to control the roughness of the thin-film during deposition process.

References

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