CENTER FOR NANOSCALE SCIENCE AND TECHNOLOGY

University of Illinois at Urbana-Champaign

Decision and Control Laboratory

Richard D. Braatz

Professor of Chemical and Biomolecular Engineering

University of Illinois at Urbana-Champaign

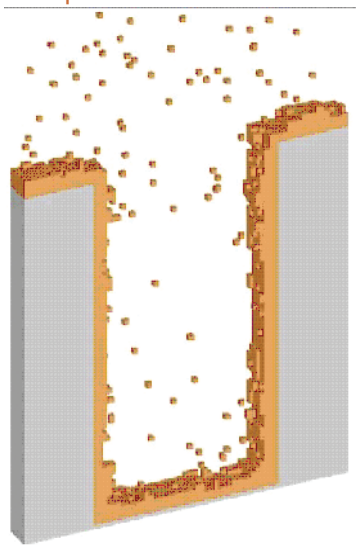
Multiscale Systems Engineering with Applications to Electronic Devices

Wednesday, October 8, 2003
4:00 p.m.
B02 Coordinated Science Laboratory
Reception to Follow

New applications in materials, medicine, and computers are being discovered where the control of events at the molecular and nanoscopic scales is critical to product quality, although the primary manipulation of these events during processing occurs at macroscopic length scales. This drives research in the creation of engineering tools for the design and control of multiscale systems that have length scales ranging from the atomistic to the macroscopic. The challenges to building such tools include uncertainties in nanoscale physics and chemistry, in terms of the physicochemical mechanisms as well as kinetic and thermodynamic parameters; complexities in the simulation of model equations that span the subatomic to the macroscopic scales; lack of direct real-time measurements of most properties at the nanoscale; and the inapplicability of most existing systems engineering tools to address systems described by dynamically coupled simulation models.

A systematic approach will be described for addressing these challenges to multiscale systems engineering, using stochastic parameter sensitivity analysis, Bayesian parameter estimation applied to ab initio calculations and experimental data, hypothesis mechanism selection, and multiscale optimal design and control. This enables multiscale systems to be designed and controlled based on the simulation codes that are most appropriate for simulating the various length scales of the process.

Coarse-grained Kinetic Monte Carlo simulation of deposition into a trench



New developments in multiscale systems engineering are driven by applications to a variety of complex chemical systems including the formation of transistor junctions in advanced CMOS devices and the manufacture of copper interconnects in electronic devices. For ultrashallow junctions, the results provide specific recommendations for microelectronics tool manufacturers on how to optimize processes to produce shallower junctions. For copper interconnects, systems principles are used to suppress numerical instabilities in multiscale simulation codes, gain fundamental insights into surface reaction mechanisms, and design nonlinear feedback controllers. Some open research problems in multiscale systems engineering will be discussed.