

Department of Applied Mathematics and Statistics
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SEMINAR

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February 2, 2006
110 Maryland Hall
Refreshments: 3:30 p.m.
(in 301 Whitehead Hall)
Seminar: 4:00 p.m.

**MORPHOLOGICAL EVOLUTION OF CRYSTAL SURFACES:
MODELING FROM THE NANOSCALE TO THE MACROSCALE**

ABSTRACT

Recent and near-future technological advances rely on the synthesis and stability of small features on crystal surfaces. This talk focuses on the derivation from microscopic considerations and applications of a continuum theory for crystal surfaces evolving below the roughening temperature. First, microscopic, discrete equations are formulated for the motion of atomic steps, which compose crystal surfaces and drive evolution, by incorporation of kinetic processes, step interactions, and material deposition from above. Second, macroscopic, continuum equations are derived from the motion of steps: The surface height profile satisfies a fourth-order, nonlinear partial differential equation (PDE) encompassing step kinetics and anisotropic effect of fluxes of point defects (“adatoms”) via the appropriate tensor mobility. Third, particular PDE solutions are invoked to plausibly unify experimental observations of decaying bi-directional profiles via an interplay of kinetics and surface topography. Fourth, the evolution of macroscopic, flat surface regions (“facets”) is described as a free-boundary problem for the PDE: The boundary conditions at facet edges must retain microscopic details and are nonlocal with time. The continuum predictions compare favorably with numerical simulations for individual step positions.