Physical Mathematics Seminar

Unified Approach to Crystal Surface Evolution Below Roughening

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Abstract

Optoelectronic devices that can revolutionize communications technology rely on the synthesis and stability of nanoscale surface structures, which have a lifetime that increases with size and decreasing temperature. At temperatures below roughening crystal surfaces have flat, macroscopic regions known as "facets" and evolve via the motion of interacting steps. This talk describes the derivation and applications of macroscopic evolution laws in (2+1) dimensions on the basis of microscopic step motion.

First, continuum evolution equations are derived from kinetic considerations accounting, for example, for diffusion of point defects ("adatoms") on terraces between arbitrarily shaped steps, and attachment and detachment of atoms at steps. The surface height outside facets is shown to satisfy a nonlinear PDE that describes adatom fluxes parallel and transverse to steps via an appropriate tensor mobility.

Second, the PDE is tested through comparisons of analytical predictions with experimental results and numerical solutions ("kinetic simulations") for the step positions. Specifically, particular solutions for the height are shown to plausibly unify experimental observations of decaying bi-directional profiles via an interplay of step kinetics, step energetics and surface topography. Also, the facet evolution of axisymmetric profiles is treated as a free-boundary problem in an effort to understand suitable boundary conditions at the facet edge: For relatively weak step interactions, singular perturbation theory is applied to self-similar shapes close to the facet; scaling laws with the step interaction strength are derived, and a universal ODE for the slope profile is derived and solved uniquely. The role of Lagrangian coordinates of motion is discussed. The results for axisymmetric shapes are found in good agreement with kinetic simulations.

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