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Crystal Surface Morphological Evolution: From Step Motion to A Continuum Theory

DIONISIOS MARGETIS, Massachusetts Institute of Technology

Modern technological advances rely on the synthesis of nanoscale surface features on crystalline materials. Despite 50 years of progress, the related evolution laws have evaded a complete theoretical description. In this talk I describe analytically the recent derivation and applications of a continuum theory in 2+1 dimensions for crystal surfaces evolving below the roughening temperature. First, microscopic laws are formulated for the motion of atomic steps, which compose crystal surfaces, by incorporating: (i) diffusion of point defects (adatoms) on each terrace between steps; (ii) atom attachment-detachment at step edges; (iii) step curvature and elastic step interactions; and (iv) material deposition from above. Second, macroscopic laws are derived from step models: The surface height satisfies a fourth-order, nonlinear PDE for the anisotropic effect of fluxes of adatoms via an appropriate tensor mobility. The continuum solutions become questionable near macroscopic, flat surface regions ("facets") and step bunches. Third, particular solutions are invoked to plausibly unify experimental observations of decaying bi-directional profiles via an interplay of step kinetics and surface topography. Fourth, free-boundary problems are solved for the facet evolution of axisymmetric crystal shapes: The appropriate boundary conditions are nonlocal with time. The continuum predictions compare favorably with numerical simulations for individual steps. The formation of step bunches is studied via suitable continuum coordinates of step motion.