Tutorial Lectures on ``Mathematical Aspects of Crystal Growth''

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Lecture 1: A tale of two scales: Fundamentals of crystal surface morphological evolution

Abstract:

The goal with this lecture is to introduce basic physical and mathematical concepts permeating epitaxial relaxation and growth. This area of research encompasses mathematically rich phenomena and at the same time is strongly driven by laboratory experiments. In materials science, the design of novel devices requires understanding how structures on crystal surfaces evolve and fluctuate across several scales, from the atomistic to the continuum. In the last few decades, considerable theoretical efforts have focused on describing the motion of crystal surfaces. In this talk, I will review a few related models and their underlying principles. First, I will introduce the main mechanisms of crystal surface motion from a physics perspective, exemplifying the role of surface diffusion. Second, I will review past theories that aim to describe crystal surface morphological evolution above and below the roughening transition temperature. Emphasis will be placed on two scales, macroscale and nanoscale, and corresponding models: (i) a thermodynamics approach, which stems from the pioneering works of Mullins, Herring and others, on the basis of a continuum surface energy; and (ii) step flow models for temperatures below the roughening transition, according to the celebrated theory of Burton, Cabrera and Frank (BCF). The latter approach invokes the motion of line defects of atomic size. A third approach involves kinetic Monte Carlo simulations, which aim to capture aspects of the atomistic scale. I will discuss merits and limitations of these points of view; and mention germane issues of modeling and analysis, thus setting the stage for the following two lectures.

Lecture 2: From discrete schemes to macroscopic evolution laws: I. Coarse graining and homogenization in epitaxial relaxation

Abstract:

In this lecture, I will focus on derivations and implications of deterministic macroscopic laws for the relaxation of crystal surface morphologies at temperatures below the roughening transition. At the nanoscale, the surface motion is described by discrete equations for the positions of steps. At the macroscale, it is plausible to use Partial Differential Equations (PDEs) for the surface height or slope. Such PDEs are usually of fourth order (under surface diffusion) and fully nonlinear. The focus of this talk will be the linkage between descriptions at the nanoscale and the macroscale, especially in 2+1 dimensions where the curvature of steps and various anisotropies play an important role. My exposition will address: (i) Basic coarse-graining techniques for the formal derivation of PDEs from discrete schemes for steps; (ii) the case of surface reconstructions, where a particular homogenization procedure is applicable; (iii) the connection of the derived PDEs to thermodynamics principles, especially to continuum singular interfacial energies; and (iv) predictions of PDEs in 2+1 dimensions on the basis of numerical simulations, and their possible implications to experiments. For a large part of this lecture, I will restrict attention to monotone step trains, in the absence of macroscopically flat surface regions (facets). Issues in the modeling of material deposition (growth) and stochastic effects will be outlined.

Lecture 3: From discrete schemes to macroscopic evolution laws: II. Crystal facets and boundary conditions

Abstract:

In this talk, I will address subtle physical and mathematical issues in the global interpretation of PDEs that govern crystal surface motion below the roughening transition. In such temperature regimes, crystal surfaces often develop macroscopically flat surface regions, called facets. The existence of facets greatly complicates the interpretation of macroscopic evolution laws, since facets usually host microscopic

phenomena not captured by continuum theories. First, I will introduce the concept of a static facet from a thermodynamics perspective with recourse to the equilibrium shapes of crystals. Second, I will discuss the evolution of facets from a macroscopic viewpoint, starting with the pioneering work of Spohn who treated facets as free boundaries. This approach is intimately connected to the subgradient formulation for macroscopic evolution PDEs. Third, I will elaborate on the nature of facets from a kinetic, microscopic viewpoint. The connection of discrete schemes for steps to macroscopic evolution laws in the presence of facets will be illustrated in this context. I will show that, in principle, the discrete schemes are not consistent with the traditional thermodynamics interpretation of the macroscopic laws. This observation alludes to interesting mathematical questions.