REVIEW ARTICLE

Geometric Evolution Laws for Thin Crystalline Films: Modeling and Numerics

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Abstract. Geometrical evolution laws are widely used in continuum modeling of surface and interface motion in materials science. In this article, we first give a brief review of various kinds of geometrical evolution laws and their variational derivations, with an emphasis on strong anisotropy. We then survey some of the finite element based numerical methods for simulating the motion of interfaces focusing on the field of thin film growth. We discuss the finite element method applied to front-tracking, phase-field and level-set methods. We describe various applications of these geometrical evolution laws to materials science problems, and in particular, the growth and morphologies of thin crystalline films.

Contents

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1   Introduction

The engineering of materials with advanced properties requires the innovative design and precise control of material microstructures at micron and nanometer scales. These microstructural patterns are often characterized by interfaces—individual interfaces or interface networks—which evolve during material treatment and manufacture [12, 57, 123]. Here interfaces are understood in a broad sense: an interface can be a geometrical surface that has no thickness—a sharp interface; it can also mean a diffuse interface that can have certain thickness, e.g., of a few atomic diameters. Common examples of material interfaces include solid-liquid boundaries in solidification where a typical example is the ice-water interface near the freezing temperature of water, solid-gas boundaries such as crystal surfaces, phase interfaces in solid-solid phase transformations such as precipitate and martensite interfaces, and domain boundaries that separate different parts of material such as grain boundaries in polycrystals and domain walls in ferromagnetic materials. Compared with those of bulk phases, the properties of material interfaces can be more and more important as the length scales in devices become smaller and smaller. Evolving interfaces therefore are a key ingredient in many problems in materials science, particularly in nanoscale science and technology, and hence require more detailed consideration than in traditional material modeling.

A class of interface problems that we are particularly interested in arise from the modeling of self-organized nanoscale structures on thin solid films. Such structures consist of a large number of spatially ordered atomic objects such as quantum dots and nanowires with narrow size distributions. They possess remarkable optical, electrical, and mechanical properties that have emerging applications in many technological areas. The nucleation, coarsening, and stabilization of such patterned nanostructures are determined largely by the process of growing thin solid films in which surface energies, surface kinetics, bulk strains, and applied fields can play important roles. Accurate and efficient modeling and simulation of growth processes and surface morphologies of thin films are therefore crucial in understanding fundamental constituent mechanisms and further helping the fabrication of self-organized nanostructures on thin films.

There are mainly two kinds of continuum models of material interfaces: sharp interface models and diffuse-interface/phase-field models. In the former, individual interfaces are tracked during their relaxation and evolution. Evolving sharp interfaces are often described by motions of geometrical surfaces that have no thickness and that move with prescribed velocities that typically depend on the interface shape. Two of such geometrical motions that have important applications in material modeling are the motion by mean curvature and that by the surface Laplacian of mean curvature. In phase-field