Instabilities and Dynamics of Crystal Surfaces under Epitaxial Growth

Location :

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The physical properties of materials and their behavior under near equilibrium conditions are well defined at macroscopic scales ; the laws of fluid motion and solid elasticity account for the dynamics of continuous media. The situation is much more involved for systems in which the microscopic scales fundamentally modify their structure at large scales. This is precisely the case of growing crystal surfaces where patterns having the scale of the nanometer develop. At these intermediate scales atomic processes, like the attachment of adatoms to steps, couple with continuous degrees of freedom, related to mass transport and elastic fields, to give a rich and original phenomenology. Under the nonequilibrium conditions created by the flux of mass (molecular beam epitaxy) and elastic stress (due for example to the misfit between the crystal structures of two species, as in the case of heteroepitaxy) various instabilities develop driving the system to a nonlinear state in which self-organized structures can appear. The theoretical investigation of the physical processes governing the nonlinear evolution of growing epitaxial films is the main goal of our research, and the general framework in which more specific problems are posed.

Problem : Coarsening of step meanders on a vicinal surface A vicinal surface is obtained by cutting a perfect crystal following a plane slightly misoriented with respect to a crystalline direction. The vicinal surface is composed by a succession of terraces, coinciding with a crystal plane, and steps of monoatomic hight. In the presence of an external mass flux incoming atoms are adsorbed at the surface. These adatoms then follow a random motion on the terraces, until they reach a step where they can be attached. The asymmetry of attachment kinetics between adatoms coming from the upper or the lower terraces, related to different energy barriers, is responsible for an instability which amplify the undulations of the initially

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straight step. The aim of this study is to analyze, using mathematical methods and numerical modeling, the nonlinear dynamics of the meandering instability. In one dimension this dynamics is characterized by a coarsening of meanders, whose size and amplitude increase following power laws in time. In two dimensions, due to the intrinsic anisotropy of the vicinal surface, the length scales in the direction parallel or perpendicular to the steps are essentially different. How does the coarsening proceed in the general case of a two dimensional vicinal surface, and how it is influenced by the presence of different lengths and time scales are interesting open questions. Understanding the meander coarsening would help in the characterization of the roughening of growing crystal surfaces.

Problem : Elastic effects in heteroepitaxy The growth by heteroepitaxy of a solid film on an underlying vicinal surface is governed by effects associated with the elastic stresses and the kinetic processes controlling the mass transport. The usual approach to describe the elastic field of solid films is not applicable to a nominally flat surface or to a vicinal surface, because of the singular nature of its surface energy. The elastic field is in fact build from the interactions of defects, like adatoms or steps. The way these microscopic interactions add to determine the distribution of stress in a growing film is not known in general. The goal of this investigation is to improve our understanding of the elastic field on a singular surface, by the study of a simple model consisting of a one dimensional train of steps of both signs. The starting point of this model is the diffusion of adatoms on the terraces and their attachment kinetics, coupled with elementary elastic interactions (adatom-step, step-step). From the consideration of these microscopic processes, it is in principle possible to obtain a closed macroscopic description, in the form of integro-differential equations for the surface height, by taking a proper continuum limit. In spite of the (relative) simplicity of this model, it contains the basic physical ingredients of coupling between growth, kinetics and elasticity, as well as the dependence of the surface energy on the geometry of the deposited solid film.

Bibliography : An excellent general reference is the book : A. Pimpinelli and J. Villain, *Physics of Crystal Growth*, (Cambridge University Press, Cambridge, 1998).

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Requirements : The candidates should have a solid formation in physics and mathematical modeling, and a good knowledge of numerical methods.