A two-scale model for epitaxial surfaces

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1 Summary

Spiral surface growth is well understood in the limit where motion of the spiral ridge is controlled by the local supersaturation of adatoms in its surrounding. In liquid epitaxial growth, however, spirals can form governed by both, transport of heat as well as solute. We propose for the first time a two-scale model of epitaxial growth which takes into account all of these transport processes assuming a separation of time scales for the transport of heat compared to that of the solutal field.

2 Introduction

The spiral morphology is known to be one of the most widespread growth morphologies for crystals with atomically flat surfaces. Growth of such crystals is due to the incorporation of new atoms at monoatomic steps in the surface. If a step is pinned at a screw dislocation (see Fig. 1), they wind around this dislocation. As a consequence a spiral forms at the surface (see Fig. 2). The dynamics of the monoatomic steps as well as the final steady-state spacing l between successive steps[1] is determined by the interplay of surface diffusion, attachment kinetics of atoms at the steps, and line tension of the steps. Recently, the observations of spiral ridges in sputtered high-temperature superconducting thin films [1] and in certain semiconductor materials grown by molecular beam epitaxy (MBE) [2] has stimulated renewed interest in spiral surface growth.

Classically this growth problem is modeled by the Burton-Cabrera-Frank (BCF) approach to surface growth [3]. According to that approach atoms are first adsorbed to the crystalline surface, where they involve in a diffusion process along the surface. During this stage these atoms are called *adatoms*. Such adatoms can either desorb from the surface with a probability $1/\tau$ per unit time, or they are incorporated into the crystal at a step and thereby contribute to its growth process. Therefore, two different growth regimes can be distinguished, which depend on the ratio of l and the diffusion length $x_s = \sqrt{D\tau}$. Here D denotes the surface diffusion constant. Regime one refers to surface growth for which desorption is fast ($x_s \ll l$). As a consequence only adatoms which are deposited near a step can be incorporated, and thus step dynamics is *local*, i.e. the step velocity is completely determined by local supersaturation and by step curvature. This regime is well understood and fully accounted for by the classical BCF theory of spiral growth [3, 4].

The second regime refers to step-flow growth at temperatures where desorption is negligible. In this regime all deposited atoms reach a step. As a consequence successive turns of the spiral are strongly coupled via adatom diffusion and step dynamics turns out to be a highly non-local free boundary problem. The steady-state growth of this regime has been investigated by approximate theories [5, 6] and by the boundary integral method [7]. Succeedingly these results have been validated by full dynamical simulations of the model equations proposed by Burton, Cabrera and Frank originally based on a phase field model [8]. Moreover, the latter dynamical simulations allowed to investigate the crossover from the local to the desorption-free limit with respect to two characteristic aspects. The first of these two aspects concerns the scaling of l, the second the approach to steady-state

[1] Equivalently one could focus on the surface slope a/l, where a is the lattice parameter.

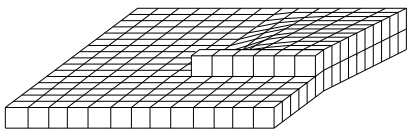

Figure 1: Dislocation at a flat surface. This dislocation might trigger spiral growth (see Fig. 2).

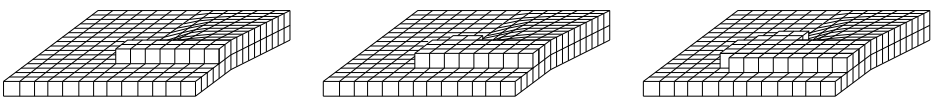

Figure 2: Step formation due to the pinning at a screw dislocation.

growth: In the local limit, spirals find their final step spacing after a single rotation. Without desorption, however, a slower relaxation to steady-state growth due to the global redistribution of adatoms is encountered. The numerical simulations in [8] reveal, that this relaxation time depends on the third power of the system size. This result refers to a surface with a single dislocation. However, it is well known that relaxation may depend on the density of screw dislocations as well.

The main goal of this contribution is to investigate spiral dynamics for a characteristic domain of a macroscopic surface containing an array of screw dislocations. I.e., we will extend the results of [8] to include the dependence on the density of screw dislocations at a surface. Doing so we will focus on the scaling of l and the relaxation to steady-state growth, as well. Our results are based on a two-scale model for surface growth, which derivation we will discuss briefly. We will then report on numerical investigations of our model resulting in our new scaling relations for dislocation growth of competing spirals. Finally we will conclude with an outlook on further applications to understand the mechanisms and consequences of spiral interaction at epitaxial surfaces in more detail.

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