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Equilibria and dislocations in epitaxial growth

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ABSTRACT

An overview of recent analytical developments in epitaxial growth is presented. The energy release via the onset of dislocations is addressed. Regularity of quasistatic equilibria is studied both in the absence and in the presence of dislocations. Morphological evolution of anisotropic epitaxially strained films is considered under the assumption that the surface evolves by surface diffusion under the influence of a chemical potential.

1. Introduction

In this paper we give an overview of recent analytical developments in the study of deposition of a crystalline film onto a substrate, in which the atoms of the film occupy natural lattice positions of the substrate. This process is called epitaxial growth. Here we are interested in heteroepitaxy, i.e., epitaxy in the case when the film and the substrate have different crystalline structures.

At the onset of the deposition the atoms of the film tend to align themselves with those of the substrate because the energy gain associated with the chemical bonding effect is greater than the strain in the film due to the mismatch between the lattice parameters. As the film continues to grow, the stored strain energy per unit area of interface increases with the film thickness, rendering the flat layer of the film morphologically unstable or metastable, after a critical value of the thickness is reached. As a result, the free surface of the film becomes corrugated and the material agglomerates into clusters or isolated islands on the substrate. The formation of islands in systems such as In-GaAs/GaAs or SiGe/Si has important applications in high-end technology such as the fabrication of modern semiconductor electronic and optoelectronic devices (quantum dots laser). The Stranski–Krastanow (SK) growth mode occurs when the islands are separated by a thin

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wetting layer, while the Volmer–Weber (VW) growth mode refers to the case when the substrate is exposed between islands.

In what follows we adopt the two dimensional variational model considered by Spencer in [44] (see also [36,45], and the references contained therein) and we follow the formulation given in [7]. We remark that two-dimensional configurations correspond to three-dimensional morphologies with planar symmetry. Although our presentation will be focused on the two-dimensional model, partial extensions of the results presented here to the three-dimensional setting can be found in [6,23].

We now describe the model more in detail. The free energy functional associated with the physical system is given by

$$\int_{\Omega_h} Q(E(u))\,dz + \int_{\Gamma_h} \psi(\nu)\,d\mathcal{H}^1, \tag{1.1}$$

where $z = (x, y) \in \mathbb{R}^2$, $h : (0, \ell) \to [0, \infty)$ is the function whose graph Γ_h describes the profile of the film, assumed to be ℓ-periodic, for some $\ell > 0$, Ω_h is the region occupied by the film, i.e.,

$$\Omega_h := \{(x, y) \in (0, \ell) \times \mathbb{R} : \, 0 < y < h(x)\},$$

$u : \Omega_h \to \mathbb{R}^2$ is displacement of the material, $E(u) := \frac{1}{2}(\nabla u + \nabla^T u)$ is the linearized strain, the elastic energy density $Q : \mathbb{M}^{2\times 2}_{\rm sym} \to [0, +\infty)$ is a positive definite quadratic form

$$Q(\xi) := \frac{1}{2}\mathbb{C}\xi : \xi,$$

with $\mathbb{C}$ a positive definite fourth-order tensor so that $Q(\xi) > 0$ for all $\xi \in \mathbb{M}^{2\times 2}_{\rm sym} \setminus \{0\}$, where : stands for the Euclidean inner product between 2×2 matrices, $\psi : \mathbb{R}^2 \to [0, \infty)$ is an anisotropic surface energy density evaluated at the unit normal ν to Γ_h, and $\mathcal{H}^1$ denotes the one-dimensional Hausdorff measure. We suppose that ψ is positively one-homogeneous and of class C^2 away from the origin, so that, in particular,

$$\frac{1}{c}|\nu| \le \psi(\nu) \le c|\nu| \quad \text{for all } \nu \in \mathbb{R}^2,$$

for some $c > 0$.

The substrate and the film admit different natural states corresponding to the mismatch between their respective crystalline structures. To be precise, a natural state for the substrate is attained at $u \equiv 0$, while a natural state for the film is given by $u \equiv A_0 z$ for some nonzero 2×2 matrix A_0. Our models will reflect this mismatch either by setting the elastic bulk energy as $\int_{\Omega_h^\infty} W\left(E\left(u\right) - E_0\right) dz$, where $\Omega_h^\infty := \{(x, y) \in (0, \ell) \times \mathbb{R} : \, y < h(x)\}$,

$$E_0(y) := \begin{cases} \dfrac{A_0 + A_0^T}{2} & \text{if } y > 0, \\ 0 & \text{if } y \le 0, \end{cases} \tag{1.2}$$

or by imposing in (1.1) the Dirichlet boundary condition of the form $u(x, 0) \equiv e_0(x, 0)$, for some constant e_0 measuring the mismatch between the lattices. In the exposition below, for the sake of presentation, we only consider the latter formulation.

The static theory to this problem was developed in [5,7,12,20,19,27] in the two-dimensional case, and in [6,9,14] in three dimensions.

In Sections 2 and 3 we study existence and regularity of equilibrium solutions of the functional (1.1) in the linearly isotropic case and when the surface energy density is $\psi \equiv 1$. In particular, we show that if the period ℓ or the thickness of the film d is sufficiently small, then the flat configuration $h = d/\ell$ is stable. Otherwise the film becomes corrugated and islands (quantum dots) are formed. In this case we can prove that the profile h is smooth except for at most a finite number of vertical cuts and cusps, which are observed experimentally for thick films. In particular, the film meets the substrate at a zero contact angle.