

Derivation of Longwave Evolution Equation for Epitaxially Strained Thin Solid Films

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Abstract

We consider a continuum model for the evolution of an epitaxially strained, dislocation-free thin solid film on a deformable substrate. In the absence of vapor deposition, we incorporate isotropic surface and strain energies along with a two-layer exponential wetting model. Applying a thin-film approximation, we successfully derive the corresponding evolution equation.

Keywords

Thin Films, Evolution Equation, Longwave Approximation

1. Introduction

Heteroepitaxial thin films are formed by depositing a single-crystal layer onto a different single-crystal substrate that shares the same crystal structure but possesses a unique lattice spacing. These films typically vary in thickness from several nanometers to a few micrometers. When subjected to epitaxial strain, they often spontaneously organize into periodic, nanoscale island structures known as quantum dots. Owing to their exceptional electronic, optical, and magnetic characteristics, these islands are widely utilized in quantum computing, data storage, and advanced optoelectronic systems [1]-[4]. To engineer highly reliable and durable devices, it is critical to understand how specific growth mechanisms govern the structural evolution of these thin layers.

Because these islands are only a few nanometers in size, they are notoriously difficult to fabricate using conventional lithographic methods. A highly promising alternative is to generate them via the Stranski-Krastanow growth mode, a process in which an initially planar film undergoes a morphological instability [5]-[8]. This type of surface roughening—driven by elastic strain and the lattice mismatch between the film and substrate—has been a subject of extensive research [9] [10].

At its core, the resulting shape transition is dictated by a competitive trade-off between strain energy and surface energy [7] [11]-[15]. Furthermore, theoretical investigations have established that the planar surface of a stressed solid film is inherently unstable, making the formation of surface undulations energetically favorable [16]-[18].

Within a thin film, cusp formation is suppressed as the moving surface approaches the film-substrate interface. The unique stress fields and differing surface energies of the film and substrate profoundly influence the surface morphology. Furthermore, provided the wetting criterion is satisfied, the film-substrate interface is prevented from being exposed, resulting instead in the formation of Stranski-Krastanov islands [19]-[22]. Numerous researchers have subsequently investigated the steady-state shapes of these islands [12] [23]-[26]. Although the theoretical frameworks and underlying modeling concepts are well advanced, implementing these models via large-scale numerical simulations remains challenging. The primary hurdle is that surface morphology dynamics are strongly coupled to the elastic strain within the system. Consequently, dynamic models must solve the elasticity equations across both the film and the substrate at every single time step—a requirement that creates severe computational bottleneck constraints for three-dimensional problems. Until recently, simulations incorporating the full elasticity problem were restricted to just one or a few islands [27]. Among recent large-scale studies, [28] examined a large population of islands by assuming identical elastic constants for both the film and substrate to simplify the mechanics. Similarly, [29] simulated numerous islands by applying a small-slope approximation restricted to the special case of an elastically rigid substrate. To address these limitations, our approach introduces a systematic, approximate solution to the elasticity problem. This method remains highly valid for thin films while successfully accommodating the general case where the film and substrate possess distinct elastic constants. The foundational thin-film methodology used here originates from the lubrication theory of viscous fluids [30]. By eliminating the need to numerically solve the complete three-dimensional elasticity equations, this formulation provides a viable path toward executing large-scale simulations. Prior work in [31] explored a comparable framework specifically for a *rigid substrate* in the absence of vapor deposition. That study demonstrated that a planar film becomes unstable once it exceeds a critical thickness, with the instability characterized by long waves at that threshold. In [32], a long-wave approximation was deployed alongside vapor deposition—but without wetting energy considerations—to model the emergence of faceted pyramidal structures. Additionally, [33] derived a nonlinear evolution equation for stress-driven morphological instability governed by surface diffusion in two-dimensional stressed solids without deposition. By obtaining a nonlinear approximation of the elastic energy density and applying numerical methods to the evolution equation, they observed a surface that evolves from small perturbations toward a cusp-like morphology. Our work distinguishes itself from these previous methodologies by directly evaluating a

coupled film-substrate system where the film and substrate can feature completely different elastic properties.

2. Model for Film Growth

Governing Equations

Figure 1 illustrates a schematic layout of the surface evolution. We build upon the model introduced by [16], which describes how surface diffusion drives the evolution of a strained film in response to elastic strain and surface energies. This formulation assumes an “atomically rough” surface. While alternative models utilize surface steps to derive the governing evolution equations [34], we restrict our focus here to the simpler case of film annealing without vapor deposition. Geometrically, the film occupies the region $0 < z < h(x, y, t)$, the substrate spans $z < 0$, and the vapor phase resides in $z > h(x, y, t)$ under zero pressure.

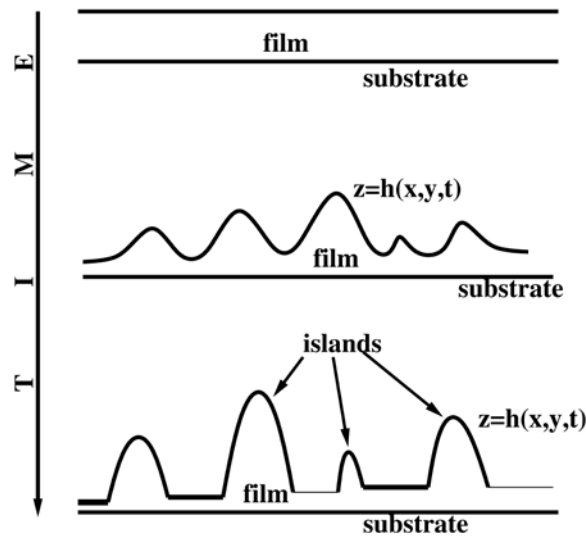


Figure 1. As time increases the originally flat film evolves to form islands.

The stress in the film and the substrate are governed by isotropic linear elasticity,

$$\sigma_{ij} = \frac{2\mu\nu}{1-2\nu} \delta_{ij} E_{kk} + 2\mu E_{ij} \quad (1)$$

where E_{ij} is the linear elasticity strain tensor given by

$$E_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i). \quad (2)$$

The variables in the governing equations are given in the following **Table 1**. Here u_i is the i^{th} Cartesian component of the displacement vector where the index $i=1,2,3$ corresponds to the x,y,z coordinates respectively, and ∂_j indicates partial derivative with respect to the j^{th} coordinate. Repeated indices imply summation from 1 to 3. The quantities $u_i, \sigma_{ij}, E_{ij}, \mu, \nu$ are defined separately in the film (F) and substrate (S). Since mechanical equilibrium exists within the

film and the substrate,

Table 1. List of symbols.

symbol	meaning
μ	elastic shear modulus
ν	Poisson's ratio
δ_{ij}	Kronecker's delta

$$\partial_j \sigma_{ij} = 0 \text{ in F, S.} \quad (3)$$

Upon substituting the formulas for stress and strain in this equation we obtain Navier's equations

$$(1-2\nu)\partial_k^2 u_i + \partial_k \partial_i u_k = 0 \text{ in F, S.} \quad (4)$$

On $z = h(x, y, t)$ the force on the film surface (the tractions due to the stress in the direction of the normal $\hat{n}$) is equal to the pressure in the vapor,

$$\sigma_{ij}^F \hat{n}_j = 0 \quad (5)$$

where

$$\hat{n} = \frac{(-h_x, -h_y, 1)}{\sqrt{1+h_x^2+h_y^2}}.$$

The substrate is taken to be semi-infinite, and so the displacements vanish far beneath the film,

$$u_i^S \rightarrow 0 \text{ as } z \rightarrow -\infty. \quad (6)$$

On $z = 0$ (the film/substrate interface), the misfit condition gives

$$u_i^F = u_i^S + \epsilon \begin{bmatrix} x \\ y \\ 0 \end{bmatrix} \quad (7)$$

where ϵ is the misfit strain in the film, induced by the lattice matching of the film to the substrate, characterized by

$$\epsilon = (a_f - a_s)/a_s \quad (8)$$

where a_f and a_s are the lattice spacings of the film and the substrate, respectively. Finally, a force balance on $z = 0$ gives

$$\sigma_{ij}^F \hat{z} = \sigma_{ij}^S \hat{z} \quad (9)$$

where $\hat{z}$ is unit vector in the z direction.

The evolution equation for the surface $z = h(x, y, t)$ is determined by surface diffusion in response to a chemical potential $\mathcal{M}$,

$$\frac{\partial h}{\partial t} = D \sqrt{1+|\nabla h|^2} \nabla_s^2 (\mathcal{M}) \quad (10)$$

where ∇_s^2 is the surface Laplacian,

$$\nabla_s^2 = \frac{1}{1+h_x^2+h_y^2} \left[(1+h_y^2)\partial_x^2 - 2h_xh_y\partial_x\partial_y + (1+h_x^2)\partial_y^2 - \frac{(1+h_y^2)h_{xx} - 2h_xh_yh_{xy} + (1+h_x^2)h_{yy}}{1+h_x^2+h_y^2} (h_x\partial_x + h_y\partial_y) \right] \quad (11)$$

D is a constant related to surface diffusion, and the surface chemical potential is

$$\mathcal{M} = \mathcal{E} + \gamma\kappa + \omega(h) \quad (12)$$

where $\mathcal{E}$ is the elastic energy density, $\gamma\kappa$ represents the surface energy, and $\omega(h)$ is the wetting energy. In the above,

$$\mathcal{E} = \frac{1}{2} \sigma_{ij}^F E_{ij}^F \quad \text{on } z = h(x, y, t) \quad (13)$$

and the curvature of the film κ is given by

$$\kappa = - \frac{(1+h_y^2)h_{xx} - 2h_xh_yh_{xy} + (1+h_x^2)h_{yy}}{(1+h_x^2+h_y^2)^{3/2}}. \quad (14)$$

3. Model for the Wetting Energy

To model the wetting energy $\omega(h)$ we use a two layer exponential form, based on a surface energy which depends on the film thickness and undergoes a rapid transition from γ_F to γ_S over a length scale δ :

$$\gamma(h) = \frac{1}{2}(\gamma_F + \gamma_S) + \frac{1}{2}(\gamma_F - \gamma_S) f(h/\delta), \quad (15)$$

which gives the wetting term,

$$\omega(h) = \hat{n}_z \gamma'(h) \quad (16)$$

where $\hat{n}_z$ is the z component of $\hat{n}$,

$$f(h/\delta) = 1 - e^{-h/\delta} \quad (17)$$

and

$$\Delta\gamma = \gamma_S - \gamma_F.$$

Hence we get

$$\omega(h) = \frac{1}{\sqrt{1+|\nabla h|^2}} \frac{\Delta\gamma}{2\delta} e^{-h/\delta}. \quad (18)$$

Equation (10) is a non-linear moving boundary problem coupled to partial differential equations for the elasticity problem (4)-(9).

4. Thin-Film Approximation and Derivations

Following the scalings, notations, and derivations presented in [35], the nondimensionalized wetting energy density is obtained as:

$$\omega(\alpha l H) \sim \frac{-\Delta\gamma}{l\pi} \frac{\tilde{\delta}}{\alpha^2 H^2} \left(1 - \frac{1}{2} \alpha^2 |\nabla H|^2 - \frac{\tilde{\delta}^2}{\alpha^2 H^2} + \dots \right). \quad (19)$$

To balance the wetting energy term $\mathcal{O}(\tilde{\delta}/\alpha^2)$ with the surface energy term $\mathcal{O}(\alpha)$ in (12) we choose

$$\tilde{\delta} = \mathcal{O}(\alpha^3)$$

and define

$$\tilde{\delta} = \delta^* \alpha^3$$

where $\delta^* = \mathcal{O}(1)$. Then defining

$$\tilde{\omega} = \frac{1}{\alpha} \frac{l}{\gamma} \omega(\alpha l H), \quad (20)$$

we obtain

$$\tilde{\omega} = \tilde{\omega}_0 + \alpha^2 \tilde{\omega}_2 + \mathcal{O}(\alpha^4) \quad (21)$$

where

$$\begin{aligned} \tilde{\omega}_0 &= \frac{-\Delta \gamma}{\pi \gamma} \frac{\delta^*}{H^2} \\ \tilde{\omega}_2 &= \frac{1}{2} \frac{-\Delta \gamma}{\pi \gamma} \frac{\delta^*}{H^2} |\nabla H|^2. \end{aligned}$$

We substitute these expansions into the evolution Equation (10) to obtain

$$\frac{\partial H}{\partial T} = \nabla^2 (\tilde{\mathcal{E}}_1 - \nabla^2 H + \tilde{\omega}_0) + \alpha \nabla^2 \tilde{\mathcal{E}}_2 + \mathcal{O}(\alpha^2) \quad (22)$$

where

$$\tilde{\mathcal{E}}_1 = \frac{l \mathcal{E}_1}{\gamma} = \frac{\mathcal{E}_1}{\mathcal{E}_0}$$

and

$$\tilde{\mathcal{E}}_2 = \frac{l \mathcal{E}_2}{\gamma} = \frac{\mathcal{E}_2}{\mathcal{E}_0}.$$

Equation (22) is the thin film evolution equation. It depends on elastic response through $\tilde{\mathcal{E}}_1$ and $\tilde{\mathcal{E}}_2$, which we now determine.

Evolution Equation

Returning to Equation (22) using the expansions derived above we get

$$\begin{aligned} \frac{\partial H}{\partial T} &= \nabla^2 (\tilde{\mathcal{E}}_1 - \nabla^2 H + \tilde{\omega}_0) + \alpha \nabla^2 \tilde{\mathcal{E}}_2 \\ &\quad + \alpha^2 \left[\nabla^2 \left(\tilde{\mathcal{E}}_3 - H_Y^2 H_{XX} + 2H_X H_Y H_{XY} - H_X^2 H_{YY} + \frac{3}{2} |\nabla H|^2 \nabla^2 H + \tilde{\omega}_2 \right) + \dots \right] + \mathcal{O}(\alpha^3) \end{aligned}$$

where

$$\tilde{\mathcal{E}}_j = F^{-1} \left[\hat{\mathcal{E}}_j \right]$$

This evolution equation is derived in a self-consistent thin film approximation. It can be used to characterize pattern formation in thin films with order of α we are interested in.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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