

Surface evolution of elastically stressed films

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An overview of recent analytical developments in the study of epitaxial growth is presented. Quasistatic equilibrium is established, regularity of solutions is addressed, and the evolution of epitaxially strained elastic films is treated using minimizing movements.

In this paper, we give a brief overview of recent analytical developments in the study of the deposition of a crystalline film onto a substrate, with the atoms of the film occupying the substrate's natural lattice positions. This process is called epitaxial growth. Here we are interested in heteroepitaxy, that is, epitaxy when the film and the substrate have different crystalline structures. At the onset of the deposition, the film's atoms tend to align themselves with those of the substrate because the energy gain associated with the chemical bonding effect is greater than the film's strain due to the mismatch between the lattice parameters. As the film continues to grow, the stored strain energy per unit area of the interface increases with the film thickness, rendering the film's flat layer morphologically unstable or metastable after the thickness reaches a critical value. As a result, the film's free surface 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 essential high-end technology applications, such as modern semiconductor electronic and optoelectronic devices (quantum dots laser). The Stranski-Krastanow (SK) growth mode occurs when the islands are separated by a thin 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 variational model considered by Spencer in [41] (see also [36, 42], and the references contained therein). To be precise, the free energy functional associated with the physical system is given by

$$\int_{\Omega_h} W(\mathbf{E}(\mathbf{u})) \, dx + \int_{\Gamma_h} \psi(\boldsymbol{\nu}) \, d\mathcal{H}^2. \quad (1)$$

Here $h : Q \rightarrow [0, \infty)$ is the function whose graph Γ_h describes the profile of the film, assumed to be Q -periodic, with

$Q := (0, b)^2 \subset \mathbb{R}^2$, for some $b > 0$, Ω_h is the region occupied by the film, i.e., writing $x = (x, y, z)$,

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

$\mathbf{u} : \Omega_h \rightarrow \mathbb{R}^3$ is displacement of the material, $\mathbf{E}(\mathbf{u}) := \frac{1}{2}(D\mathbf{u} + D^T\mathbf{u})$ is the symmetric part of $D\mathbf{u}$. Also, the elastic energy density $W : \mathbb{M}_{\text{sym}}^{3 \times 3} \rightarrow [0, +\infty)$ is a positive definite quadratic form defined on the space of 3×3 symmetric matrices

$$W(A) := \frac{1}{2} \mathbb{C}A : A,$$

with \mathbb{C} a positive definite fourth-order tensor, so that $W(A) > 0$ for all $A \in \mathbb{M}_{\text{sym}}^{3 \times 3} \setminus \{0\}$, $\psi : \mathbb{R}^3 \rightarrow [0, \infty)$ is an anisotropic surface energy density evaluated at the unit normal $\boldsymbol{\nu}$ to Γ_h , and \mathcal{H}^2 denotes the two-dimensional Hausdorff measure. We suppose that ψ is positively one-homogeneous and of class C^2 away from the origin, so that, in particular,

$$\frac{1}{c}|\boldsymbol{\xi}| \leq \psi(\boldsymbol{\xi}) \leq c|\boldsymbol{\xi}| \quad \text{for all } \boldsymbol{\xi} \in \mathbb{R}^3,$$

for some constant $c > 0$.

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 given by $\mathbf{u} \equiv \mathbf{0}$, while a natural state for the film is given by $\mathbf{u} \equiv \mathbf{A}_0 \mathbf{x}$ for some nonzero 3×3 matrix \mathbf{A}_0 . Our models will reflect this mismatch, either by setting the elastic bulk energy as $\int_{\Omega_h} W(\mathbf{E}(\mathbf{u}))(\mathbf{x}) - E_0(\mathbf{x}) \, dx$, where

$$E_0(\mathbf{x}) := \begin{cases} \frac{A_0 + A_0^T}{2} & \text{if } z > 0, \\ \mathbf{0} & \text{if } z \leq 0, \end{cases} \quad (2)$$

or by imposing the Dirichlet boundary condition $\mathbf{u}(x, y, 0) \equiv \mathbf{A}_0(x, y, 0)$.

In the two-dimensional static case, existence of equilibrium solutions and their qualitative properties, including regularity, were studied in [3, 4, 5, 15, 16, 17, 20, 24, 26, 29, 33]. The variational techniques and analytical arguments developed in these papers have been used to treat other materials phenomena, such as voids and cavities in elastic solids [9, 19].

The scaling regimes of the minimal energy in epitaxial growth were identified in [2, 30] in terms of the parameters of the problem. The shape of the islands under the constraint of faceted profiles

was addressed in [25]. A variational model that takes into account the formation of misfit dislocations was introduced in [23].

The effect of atoms freely diffusing on the surface (called adatoms) was studied in [10], where the model involves only surface energies.

A discrete-to-continuum analysis for free-boundary problems related to crystalline films deposited on substrates was undertaken in [35, 38].

The three-dimensional static case was studied in [6, 12] in the case in which the symmetrized gradient $E(u)$ is replaced by the gradient (see also [4]). More recently, new developments in the theory of *GSBD*, i.e., generalized special functions of bounded deformation (see [13, 14], and the references therein) have led to considerable progress on the relaxation of the functional (1) in the three dimensional case (see [13]). The regularity of equilibrium solutions remains an open problem. A local minimality sufficiency criterion, based on the strict positivity of the second variation, was established in [4], based on the work [29].

To study the morphological evolution of anisotropic epitaxially strained films, we assume that the surface evolves by *surface diffusion* under the influence of a chemical potential μ . To be precise, according to the Einstein–Nernst relation, the evolution is governed by the *volume preserving* equation

$$V = C\Delta_\Gamma\mu, \quad (3)$$

where $C > 0$, V denotes the normal velocity of the evolving interface Γ , Δ_Γ stands for the tangential laplacian, and the chemical potential μ is given by the first variation of the underlying free-energy functional. In our context, this becomes (assuming $C = 1$)

$$V = \Delta_\Gamma[\operatorname{div}_\Gamma(D\psi(\nu)) + W(E(u))], \quad (4)$$

where $\operatorname{div}_\Gamma$ stands for the tangential divergence along $\Gamma_{h(\cdot,t)}$, and $u(\cdot, t)$ is the elastic equilibrium in $\Omega_{h(\cdot,t)}$, i.e., the minimizer of the elastic energy under the prescribed periodicity and boundary conditions (see (7) below).

If the surface energy density ψ is highly anisotropic, there may be directions ν for which

$$D^2\psi(\nu)[\tau, \tau] > 0 \quad \text{for all } \tau \perp \nu, \tau \neq 0$$

fails, see for instance [18, 40]. In this case, the evolution equation (4) is backward parabolic, and to overcome the ill-posedness of the problem we consider the following singular perturbation of the surface energy

$$\int_{\Gamma_h} \left(\psi(\nu) + \frac{\varepsilon}{p} |H|^p \right) d\mathcal{H}^2,$$

where $p > 2$, H stands for the sum $\kappa_1 + \kappa_2$ of the principal curvatures of Γ_h , and ε is a small positive constant (see [18, 31, 32]). The restriction $p > 2$ in \mathbb{R}^3 is motivated by the fact that the profile h of the film will belong to $W^{2,p}(Q)$, where $Q \subset \mathbb{R}^2$, so that $W^{2,p}(Q)$ is continuously embedded into $C^{1, \frac{p-2}{p}}(Q)$. This regularity is strongly

used to prove existence of solutions. In contrast, in \mathbb{R}^2 we can assume $p \geq 2$ since $W^{2,2}((0, b))$ is embedded in $C^{1,1}([0, b])$.

The regularized free-energy functional becomes

$$\int_{\Omega_h} W(E(u)) dx + \int_{\Gamma_h} \left(\psi(\nu) + \frac{\varepsilon}{p} |H|^p \right) d\mathcal{H}^2, \quad (5)$$

and (3) is replaced by

$$V = \Delta_\Gamma \left[\operatorname{div}_\Gamma(D\psi(\nu)) + W(E(u)) - \varepsilon \left(\Delta_\Gamma(|H|^{p-2}H) - |H|^{p-2}H \left(\kappa_1^2 + \kappa_2^2 - \frac{1}{p} H^2 \right) \right) \right]. \quad (6)$$

Coupling this evolution equation on the profile of the film with the elastic equilibrium elliptic system holding in the film, and parametrizing Γ using $h : \mathbb{R}^2 \times [0, T_0] \rightarrow (0, \infty)$, we obtain the following Cauchy system of equations with initial and natural boundary conditions:

$$\begin{cases} \frac{1}{J} \frac{\partial h}{\partial t} = \Delta_\Gamma \left[\operatorname{div}_\Gamma(D\psi(\nu)) + W(E(u)) - \varepsilon \left(\Delta_\Gamma(|H|^{p-2}H) - |H|^{p-2}H \left(\kappa_1^2 + \kappa_2^2 - \frac{1}{p} H^2 \right) \right) \right] \\ \quad \text{in } \mathbb{R}^2 \times (0, T_0), \\ \operatorname{div} CE(u) = 0 \text{ in } \Omega_h, \\ CE(u)[\nu] = 0 \text{ on } \Gamma_h, \quad u(x, y, 0, t) = A_0(x, y, 0), \\ h(\cdot, t) \text{ and } Du(\cdot, t) \text{ are } Q\text{-periodic,} \\ h(\cdot, 0) = h_0, \end{cases} \quad (7)$$

where $J := \sqrt{1 + |Dh|^2}$ and $h_0 \in H_{\text{loc}}^2(\mathbb{R}^2)$ is a Q -periodic function.

One can find in the literature sixth-order evolution equations of this type (see, e.g., [31] for the case without elasticity, see [40] for the evolution of voids in elastically stressed materials, and [7, 39]).

We use the gradient flow structure of (7) with respect to a suitable H^{-1} -metric (see, e.g., [8]) to solve the equation via a *minimizing movement scheme* (see [1]), i.e., we discretize the problem in time and solve suitable minimum incremental problems.

If instead of H^{-1} we used the gradient flow with respect to an L^2 -metric, we would obtain a fourth order evolution equation describing motion by evaporation-condensation (see [8, 31, 37]).

The short time existence of solutions to (7) established in [22] is the first such result for geometric surface diffusion equations with elasticity in three-dimensions. In the recent paper [28] (see also [27] for the two-dimensional case), the authors proved short-time existence of a smooth solution without the additional curvature regularization. They also showed asymptotic stability of strictly stable stationary sets.

The results summarized here can be found in the papers [20, 21, 22].

1 2D quasistatic equilibrium of epitaxially strained elastic films

In the following sections we assume self-similarity with respect to a planar axis and reduce the context to a two-dimensional framework. To be precise, we suppose that the material fills the infinite strip

$$\Omega_h := \{x = (x, y) : 0 < x < b, y < h(x)\}, \quad (8)$$

where $h : [0, b] \rightarrow [0, \infty)$ is a Lipschitz function representing the free profile of the film, which occupies the open set

$$\Omega_h^+ := \Omega_h \cap \{y > 0\}. \quad (9)$$

The line $y = 0$ corresponds to the film/substrate interface.

We assume that the mismatch strain corresponding to different natural states of the material in the substrate and in the film, respectively, is represented by

$$E_0(y) = \begin{cases} \hat{E}_0 & \text{if } y \geq 0, \\ 0 & \text{if } y < 0, \end{cases} \quad (10)$$

with $\hat{E}_0 \neq \mathbf{0} > 0$. We will suppose that the film and the substrate share material properties, with homogeneous elasticity positive definite fourth-order tensor \mathbb{C} . Hence, bearing in mind the mismatch, the elastic energy per unit area is given by $W(E - E_0(y))$, where

$$W(E) := \frac{1}{2} E \cdot \mathbb{C}[E] \quad (11)$$

for all symmetric matrices $E \neq \mathbf{0}$.

In turn, the interfacial energy density ψ has a step discontinuity at $y = 0$, i.e.,

$$\psi(y) := \begin{cases} \gamma_{\text{film}} & \text{if } y > 0, \\ \gamma_{\text{sub}} & \text{if } y = 0, \end{cases} \quad (12)$$

where the property

$$\gamma_{\text{sub}} \geq \gamma_{\text{film}} > 0 \quad (13)$$

will favor the SK growth mode over the VW mode. For the case $\gamma_{\text{sub}} < \gamma_{\text{film}}$, and for different crystalline materials stress tensors \mathbb{C} for the substrate and for the film, we refer to [15, 16].

The total energy of the system is given by

$$\mathcal{F}(u, h) := \int_{\Omega_h} W(E(u) - E_0) dx + \int_{\Gamma_h} \psi ds, \quad (14)$$

where Γ_h represents the free surface of the film, that is,

$$\Gamma_h := \partial\Omega_h \cap ((0, b) \times \mathbb{R}). \quad (15)$$

Since the functional \mathcal{F} is not lower semicontinuous, and thus, in general, does not admit minimizers, we are led to study its relaxation. Let

$$X := \left\{ (u, h) : h : [0, b] \rightarrow [0, \infty) \text{ Lipschitz,} \right. \\ \left. \int_0^b h dx = d, \quad u \in H_{\text{loc}}^1(\Omega_h; \mathbb{R}^2) \right\}$$

and

$$X_0 = \left\{ (u, h) : h : [0, b] \rightarrow [0, \infty) \text{ lower semicontinuous,} \right. \\ \left. \text{var}_{[0, b]} h < \infty, \quad \int_0^b h dx = d, \quad u \in H_{\text{loc}}^1(\Omega_h; \mathbb{R}^2) \right\},$$

where $\text{var}_{[0, b]} h$ stands for the pointwise variation of the function h . Note that length Γ_h coincides with the pointwise variation of the function $x \in [0, b] \mapsto (x, h(x))$, and so

$$\text{var}_{[0, b]} h \leq \text{length } \Gamma_h \leq b + \text{var}_{[0, b]} h. \quad (16)$$

For $(u, h) \in X_0$ define

$$\mathcal{G}(u, h) := \int_{\Omega_h} W(E(u)(x) - E_0(y)) dx + \gamma_{\text{film}} \text{length } \Gamma_h. \quad (17)$$

Theorem 1 (Existence). *The following equalities hold:*

$$\inf_{(u, h) \in X} \mathcal{F}(u, h) = \inf_{(u, h) \in X_0} \mathcal{G}(u, h) = \min_{(u, h) \in X_0} \mathcal{G}(u, h).$$

We refer to [20] for a proof.

Next we study regularity properties of minimizers of \mathcal{G} in X_0 . As customary in constrained variational problems, in order to have more flexibility in the choice of test functions, we prove that the volume constraint $\int_0^b h(x) dx = d$ can be replaced by a volume penalization.

Theorem 2 (Volume penalization). *Let $(u_0, h_0) \in X_0$ be a minimizer of the functional \mathcal{G} defined in (17) with $\int_0^b h_0(x) dx = d$. Then there exists $k_0 \in \mathbb{N}$ such that for every integer $k \geq k_0$, (u_0, h_0) is a minimizer of the penalized functional*

$$\mathcal{G}_k(u, h) := \int_{\Omega_h} W(E(u) - E_0) dx + \gamma_{\text{film}} \text{length } \Gamma_h + k \left| \int_0^b h dx - d \right| \quad (18)$$

over all $(u, h) \in X_0$.

Proof. An argument similar to that of the proof of Theorem 1 guarantees that for every $k \in \mathbb{N}$ there exists a minimizer (v_k, f_k) of \mathcal{G}_k . If $\int_0^b f_k dx = d$ for all k sufficiently large, then

$$\mathcal{G}(u_0, h_0) \leq \mathcal{G}(v_k, f_k) = \mathcal{G}_k(v_k, f_k) \leq \mathcal{G}_k(u_0, h_0) = \mathcal{G}(u_0, h_0) < \infty,$$

and so (u_0, h_0) is a minimizer of \mathcal{G}_k .

Assume now that there is a subsequence, not relabeled, such that $\int_0^b f_k dx \neq d$ for all k . If

$$\int_0^b f_k dx > d \quad (19)$$

for countably many k , define

$$h_k := \min\{f_k, t_k\},$$

where $t_k > 0$ has been chosen so that $\int_0^b h_k dx = d$. Note that $\text{length } \Gamma_{h_k} \leq \text{length } \Gamma_{f_k}$. Indeed, for every partition $x_0 = 0 < \dots < x_n = b$, we have that

$$(h_k(x_i) - h_k(x_{i-1}))^2 \leq (f_k(x_i) - f_k(x_{i-1}))^2$$

for all $i = 1, \dots, n$. Hence,

$$\mathcal{G}(v_k, h_k) = \mathcal{G}_k(v_k, h_k) < \mathcal{G}_k(v_k, f_k),$$

which is a contradiction. Therefore, for all k sufficiently large

$$\int_0^b f_k dx < d.$$

Since

$$\mathcal{G}_k(v_k, f_k) \leq \mathcal{G}_k(u_0, h_0) = \mathcal{G}(u_0, h_0) < \infty, \quad (20)$$

it follows from (18) and (20) that $\int_0^b f_k dx \rightarrow d$ as $k \rightarrow \infty$ and that $\sup_k \text{length } \Gamma_{f_k} < \infty$. In turn, by (16), $\|f_k\|_\infty \leq c$ for some constant c independent of k .

Let k_1 be so large that $\int_0^b f_k dx > \frac{d}{2}$ for all $k \geq k_1$. Then

$$t_k := \frac{d}{\int_0^b f_k dx} \in (0, 2)$$

and the function $h_k(x) := t_k f_k(x)$, $x \in (0, b)$, satisfies

$$\int_0^b h_k dx = d.$$

Consider a partition $0 = x_0 < \dots < x_\ell = b$. Then

$$\begin{aligned} & \sum_{i=1}^{\ell} \sqrt{(x_i - x_{i-1})^2 + (h_k(x_i) - h_k(x_{i-1}))^2} \\ &= \sum_{i=1}^{\ell} \sqrt{(x_i - x_{i-1})^2 + t_k^2 (f_k(x_i) - f_k(x_{i-1}))^2} \\ &\leq t_k \sum_{i=1}^{\ell} \sqrt{(x_i - x_{i-1})^2 + (f_k(x_i) - f_k(x_{i-1}))^2} \\ &\leq t_k \text{length } \Gamma_{f_k}, \end{aligned}$$

where we used the fact that $t_k > 1$. Hence,

$$\text{length } \Gamma_{h_k} \leq t_k \text{length } \Gamma_{f_k},$$

and so, by (20),

$$\begin{aligned} \gamma_{\text{film}} \text{length } \Gamma_{h_k} - \gamma_{\text{film}} \text{length } \Gamma_{f_k} \\ \leq (t_k - 1) \gamma_{\text{film}} \text{length } \Gamma_{f_k} \leq (t_k - 1) \mathcal{G}_k(v_k, f_k) \\ \leq (t_k - 1) \mathcal{G}(u_0, h_0). \end{aligned}$$

We deduce that

$$\gamma_{\text{film}} \text{length } \Gamma_{h_k} \leq \gamma_{\text{film}} \text{length } \Gamma_{f_k} + (t_k - 1) \mathcal{G}(u_0, h_0). \quad (21)$$

For $(x, y') \in \Omega_{h_k}$ define

$$w_k(x, y') := \left((v_k)_1 \left(x, \frac{y'}{t_k} \right), \frac{1}{t_k} (v_k)_2 \left(x, \frac{y'}{t_k} \right) \right).$$

By a change of variables and (10), we have

$$\begin{aligned} \int_{\Omega_{h_k}} W(E(w_k)(x, y') - E_0(y')) dx dy' \\ = \frac{1}{t_k} \int_{\Omega_{f_k}} W(\tilde{E}(v_k)(x) - E_0(y)) dx, \end{aligned}$$

where $\tilde{E}(v_k)(x)$ is the 2×2 matrix whose entries are

$$\begin{aligned} \tilde{E}_{11}(v_k)(x) &= E_{11}(v_k)(x), & \tilde{E}_{12}(v_k)(x) &= \frac{1}{t_k} E_{12}(v_k)(x), \\ \tilde{E}_{22}(v_k)(x) &= \frac{1}{t_k^2} E_{22}(v_k)(x). \end{aligned} \quad (22)$$

Observe that

$$\begin{aligned} (|\tilde{E}(v_k) - E_0| + |E(v_k) - E_0|) |\tilde{E}(v_k) - E(v_k)| \\ \leq c(t_k - 1) (|\tilde{E}(v_k) - E_0| + |E(v_k) - E_0|) |E(v_k)| \\ \leq c(t_k - 1) (|E(v_k)| + |E_0|) (|E(v_k) - E_0| + |E_0|) \\ \leq c(t_k - 1) (|E(v_k) - E_0| + |E_0|)^2. \end{aligned} \quad (23)$$

Since $W(E)$ is a positive definite quadratic form over the 2×2 symmetric matrices (see (11)), we have that

$$|W(E) - W(E_1)| \leq c(|E| + |E_1|) |E - E_1|$$

for all 2×2 symmetric matrices E and E_1 . Hence by (1), (10) and (23)

$$\begin{aligned} \int_{\Omega_{h_k}} W(E(w_k)(x, y') - E_0(y')) dx' - \int_{\Omega_{f_k}} W(E(v_k)(x) - E_0(y)) dx \\ = \frac{1}{t_k} \int_{\Omega_{f_k}} [W(\tilde{E}(v_k)(x) - E_0(y)) - W(E(v_k)(x) - E_0(y))] dx \\ \leq c \int_{\Omega_{f_k}} (|\tilde{E}(v_k) - E_0| + |E(v_k) - E_0|) (|\tilde{E}(v_k) - E(v_k)|) dx \\ \leq c(t_k - 1) \int_{\Omega_{f_k}} (|E(v_k) - E_0| + |E_0|)^2 dx \\ \leq c(t_k - 1) (\mathcal{G}_k(v_k, f_k) + |\hat{E}_0|^2) \leq c(t_k - 1) (\mathcal{G}(u_0, h_0) + |\hat{E}_0|^2), \end{aligned} \quad (24)$$

where c depends only on the ellipticity constants of W and $\sup_k \|f_k\|_\infty$. By (20), (21), and (24), we have that

$$\begin{aligned} \mathcal{G}(u_0, h_0) \\ \leq \mathcal{G}(w_k, h_k) \leq \mathcal{G}(v_k, f_k) + (t_k - 1) \left[(c + 1) \mathcal{G}(u_0, h_0) + c |\hat{E}_0|^2 \right] \\ = \mathcal{G}_k(v_k, f_k) + (t_k - 1) \left[(c + 1) \mathcal{G}(u_0, h_0) + c |\hat{E}_0|^2 \right] \\ \quad - k \left(d - \int_0^b f_k dx \right) \\ = \mathcal{G}_k(v_k, f_k) + (t_k - 1) \left[(c + 1) \mathcal{G}(u_0, h_0) + c |\hat{E}_0|^2 \right] \\ \quad - (t_k - 1) k \int_0^b f_k dx \\ \leq \mathcal{G}(u_0, h_0) + (t_k - 1) \left[(c + 1) \mathcal{G}(u_0, h_0) + c |\hat{E}_0|^2 - k \frac{d}{2} \right]. \end{aligned}$$

Thus, if

$$k \geq \frac{2}{d} \left[(c + 1) \mathcal{G}(u_0, h_0) + c |\hat{E}_0|^2 \right] + 1,$$

we get a contradiction, and this completes the proof. ■

To prove the regularity of the free boundary we use the following internal sphere condition.

Theorem 3 (Internal Sphere's Condition). *Let $(u_0, h_0) \in X_0$ be a minimizer of the functional \mathcal{G} defined in (17). Then there exists $r_0 > 0$ with the property that for every $z_0 \in \bar{\Gamma}_{h_0}$ there exists an open ball $B(x_0, r_0)$, with $B(x_0, r_0) \cap ((0, b) \times \mathbb{R}) \subseteq \Omega_{h_0}$, such that*

$$\partial B(x_0, r_0) \cap \bar{\Gamma}_{h_0} = \{z_0\}.$$

This result was first proved in a slightly different context by Chambolle and Larsen [11] (see also [9, 20]). The argument is entirely two-dimensional and its extension to three dimensions is open.

Remark 4. Note that if $\nu_0 \in \partial B(\mathbf{0}, 1)$ is the outward unit normal to $B(x_0, r_0)$ at z_0 , then $x_0 = z_0 - r_0 \nu_0$. Thus, the set

$$N_{z_0} := \{\nu \in \partial B(\mathbf{0}, 1) : B(z_0 - r_0 \nu, r_0) \cap ((0, b) \times \mathbb{R}) \subseteq \Omega_{h_0}\} \quad (25)$$

is nonempty.

In the next theorem we prove that h_0 admits a left and right derivative at all but countably many points.

Theorem 5 (Left and Right Derivatives of h). *Let $(u_0, h_0) \in X_0$ be a minimizer of the functional \mathcal{G} defined in (17). Then $\bar{\Gamma}_{h_0}$ admits a left and a right tangent at every point z not of the form $z = (x, h_0(x))$ with $x \in S$, where*

$$S := \left\{x \in (0, b) : h_0(x) < \liminf_{t \rightarrow x} h_0(t)\right\}. \quad (26)$$

Define

$$\Gamma_{\text{cusps}} := \left\{z \in \bar{\Gamma}_{h_0} : \pm e_1 \in N_z\right\} \quad (27)$$

and

$$\Gamma_{\text{cuts}} := \left\{(x, y) : x \in (0, b) \cap S, h_0(x) \leq y \leq \liminf_{t \rightarrow x} h_0(t)\right\}, \quad (28)$$

where N_z is the set defined in (25) and S is the set defined in (26).

Theorem 6 (Cusps and Cuts). *Let $(u_0, h_0) \in X_0$ be a minimizer of the functional \mathcal{G} defined in (17). Then the sets Γ_{cusps} and Γ_{cuts} contain at most finitely many vertical segments.*

Remark 7. If $-e_1 \in N_{z_0}$, then since $B((x_0 + r_0, y_0), r_0) \cap ((0, b) \times \mathbb{R}) \subseteq \Omega_{h_0}$ and h_0 is lower semicontinuous, for all $x > x_0$ sufficiently close to x_0 , we have that

$$h_0(x) \geq y_0 + \sqrt{r_0^2 - (x - (x_0 + r_0))^2},$$

and so

$$\frac{h_0(x) - y_0}{x - x_0} \geq \frac{\sqrt{2r_0 - (x - x_0)}}{\sqrt{x - x_0}} \rightarrow \infty$$

as $x \rightarrow x_0^+$. By Theorem 5 it follows that $\bar{\Gamma}_{h_0}$ admits a right vertical tangent at z_0 . Similarly, if $e_1 \in N_{z_0}$ then for $x < x_0$, $\bar{\Gamma}_{h_0}$ admits a left vertical tangent at z_0 . In particular, if $\pm e_1 \in N_{z_0}$ and h_0 is continuous at x_0 , then

$$(h_0)'_-(x_0) = -\infty, \quad (h_0)'_+(x_0) = \infty. \quad (29)$$

The next theorem shows that, except for cut and cusp points, $\bar{\Gamma}_{h_0}$ is locally Lipschitz.

Theorem 8. *Let $(u_0, h_0) \in X_0$ be a minimizer of the functional \mathcal{G} defined in (17). If $z_0 \in \bar{\Gamma}_{h_0} \setminus (\Gamma_{\text{cuts}} \cup \Gamma_{\text{cusps}})$, then $\bar{\Gamma}_{h_0}$ is Lipschitz in a neighborhood of z_0 .*

In order to improve the regularity results for h , we restrict our attention to the linearly isotropic case in which

$$W(E) = \frac{1}{2} \lambda [\text{tr}(E)]^2 + \mu \text{tr}(E^2), \quad (30)$$

where λ and μ are the (constant) Lamé moduli with

$$\mu > 0, \quad \mu + \lambda > 0. \quad (31)$$

Note that in this range, the quadratic form W is coercive. We also assume that the matrix \hat{E}_0 in (10) takes the form

$$\hat{E}_0 = \begin{pmatrix} e_0 & 0 \\ 0 & 0 \end{pmatrix} \quad (32)$$

for some $e_0 > 0$, which measures the mismatch between the lattices of the two materials.

Since h_0 is now Lipschitz with left and right derivatives at all but, at most, a finite number of points, we can now obtain classical decay estimates for the solution u_0 . In turn, these will exclude corners in the graph Γ_{h_0} of h_0 .

Theorem 9 (Decay Estimate). *Assume (30) and (32). Let $(u_0, h_0) \in X_0$ be a minimizer of the functional \mathcal{G} defined in (17). Suppose that $\bar{\Gamma}_{h_0}$ has a corner at some point $z_0 \in \bar{\Gamma}_{h_0} \setminus (\Gamma_{\text{cusps}} \cup \Gamma_{\text{cuts}})$. Then there exist a constant $c > 0$, a radius r_0 , and an exponent $\frac{1}{2} < \alpha < 1$ such that*

$$\int_{B(z_0, r) \cap \Omega_{h_0}} |\nabla u_0|^2 dx \leq cr^{2\alpha} \quad (33)$$

for all $0 < r < r_0$.

Using the previous decay estimate, it can be shown that for $(u_0, \Omega) \in X$ the upper boundary $\bar{\Gamma}_{h_0}$ is of class C^1 away from $\Gamma_{\text{cusps}} \cup \Gamma_{\text{cuts}}$.

Theorem 10 (C^∞ Regularity of Γ). *Assume (30) and (32). Let $(u_0, h_0) \in X_0$ be a minimizer of the functional \mathcal{G} defined in (17). Then $\bar{\Gamma}_{h_0} \setminus (\Gamma_{\text{cusps}} \cup \Gamma_{\text{cuts}})$ is of class C^1 .*

Theorem 10 can be significantly improved. Indeed, using another blow-up argument it is possible to show that $\bar{\Gamma}_{h_0} \setminus (\Gamma_{\text{cusps}} \cup \Gamma_{\text{cuts}})$ is of class $C^{1,\alpha}$ for all $0 < \alpha < \frac{1}{2}$. In turn, this implies that \mathbf{u}_0 is of class $C^{1,\beta}$ for some $\beta > 0$ away from the x -axis and from $\Gamma_{\text{cusps}} \cup \Gamma_{\text{cuts}}$. By a classical bootstrap argument, one can obtain C^∞ regularity and then use results of [34] by Koch, Morini and the second author to prove analyticity of $\bar{\Gamma}_{h_0} \setminus (\Gamma_{\text{cusps}} \cup \Gamma_{\text{cuts}})$ away from the x -axis. We refer to [20] for more details.

2 Evolution of epitaxially strained elastic films: The 2D case

The evolution of epitaxially strained elastic films depends strongly on the possible anisotropy of the surface energy density. For this reason, in (17) we replace the isotropic surface energy γ_{film} length Γ_h by

$$\int_{\Gamma_h} \psi(\mathbf{v}) d\mathcal{H}^1,$$

where $\psi : \mathbb{R}^2 \rightarrow [0, \infty)$ is a positively one-homogeneous function of class C^2 away from the origin. Also, the mismatch between the substrate and film crystalline structures is represented by the Dirichlet condition (see (32))

$$\mathbf{u}(x, 0) = (e_0 x, 0) \quad \text{for all } x \in (0, b).$$

As discussed in the introduction, strong anisotropy of ψ may lead to the ill-posedness of the evolution law, and thus we add a higher order regularizing term. To be precise, for $\varepsilon > 0$ small the energy under study becomes

$$\mathcal{J}(\mathbf{u}, h) := \int_{\Omega_h} W(\mathbf{E}(\mathbf{u})) dx + \int_{\Gamma_h} \left(\psi(\mathbf{v}) + \frac{\varepsilon}{2} k^2 \right) d\mathcal{H}^1, \quad (34)$$

where k denotes the curvature of Γ_h and \mathbf{v} is the outer unit normal to Ω_h .

We consider periodicity conditions. Hence, given a positive b -periodic function $h : \mathbb{R} \rightarrow [0, +\infty)$, with locally finite pointwise variation, we set

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

and

$$\Gamma_h^\# := \{x = (x, y) : x \in \mathbb{R}, y = h(x)\}.$$

Given $h \in W_{\#}^{2,2}((0, b); \mathbb{R}^2)$, where $W_{\#}^{2,2}((0, b); \mathbb{R}^2)$ is the space of b periodic functions in $W_{\text{loc}}^{2,2}(\mathbb{R}; \mathbb{R}^2)$, we denote

$$X_{\#}(\Omega_h; \mathbb{R}^2) := \left\{ \mathbf{u} \in L_{\text{loc}}^2(\Omega_h^\#; \mathbb{R}^2) : \mathbf{u}(x, y) = \mathbf{u}(x+b, y) \right. \\ \left. \text{for } (x, y) \in \Omega_h^\#, \mathbf{E}(\mathbf{u})|_{\Omega_h} \in L^2(\Omega_h; \mathbb{R}^2) \right\}$$

and

$$X_{e_0} := \left\{ (\mathbf{u}, h) : h \in W_{\#}^{2,2}((0, b); \mathbb{R}^2), \right. \\ \left. \mathbf{u} \in e_0(\cdot, 0) + LD_{\#}(\Omega_h; \mathbb{R}^2), \right. \\ \left. \text{and } \mathbf{u}(x, 0) = (e_0 x, 0) \text{ for all } x \in \mathbb{R} \right\}.$$

We next introduce the incremental minimum problems used to define the discrete time evolutions. This will lead to the existence of solutions for the evolution equation (40) below via minimizing movements. Let $(\mathbf{u}_0, h_0) \in X_{e_0}$ be such that

$$h_0 > 0, \quad (35)$$

and \mathbf{u}_0 minimizes the elastic energy in Ω_{h_0} among all \mathbf{u} with $(\mathbf{u}, h_0) \in X_{e_0}$. Given $T > 0, N \in \mathbb{N}$, we set $\Delta T := \frac{T}{N}$. For $i = 1, \dots, N$, we define inductively $(\mathbf{u}_{i,N}, h_{i,N})$ as a solution of the minimum problem

$$\min \left\{ \mathcal{J}(\mathbf{u}, h) \right. \\ \left. + \frac{1}{2\Delta T} \int_{\Gamma_{h_{i-1,N}}} \left(\int_0^x (h(\zeta) - h_{i-1,N}(\zeta)) d\zeta \right)^2 d\mathcal{H}^1(x, y) : \right. \\ \left. (\mathbf{u}, h) \in X_{e_0}, \quad \|h'\|_{\infty} \leq \Lambda_0, \quad \int_0^b h dx = \int_0^b h_0 dx, \right. \\ \left. \int_{\Gamma_{h_{i-1,N}}} \int_0^x (h(\zeta) - h_{i-1,N}(\zeta)) d\zeta d\mathcal{H}^1(x, y) = 0 \right\}, \quad (36)$$

where $\|h'_0\|_{\infty} < \Lambda_0$.

Then for $x \in \mathbb{R}$ and $(i-1)\Delta T \leq t \leq i\Delta T, i = 1, \dots, N$, we set

$$h_N(x, t) := h_{i-1,N}(x) + \frac{1}{\Delta T} (t - (i-1)\Delta T) (h_{i,N}(x) - h_{i-1,N}(x)), \quad (37)$$

and we let $\mathbf{u}_N(\cdot, t)$ be the *elastic equilibrium corresponding to $h_N(\cdot, t)$, i.e., the minimizer of the elastic energy in $\Omega_{h_N(\cdot, t)}$ among all \mathbf{u} such that $(h_N(\cdot, t), \mathbf{u}) \in X_{e_0}$.*

We remark the incremental minimum problem can be written as

$$\min \left\{ \mathcal{J}(\mathbf{u}, h) + \frac{1}{2\Delta T} \left\| \frac{h - h_{i-1,N}}{\sqrt{1 + h_{i-1,N}^2}} \right\|_{H^{-1}(\Gamma_{i-1,N})}^2 : (\mathbf{u}, h) \in X_{e_0}, \right. \\ \left. \|h'\|_{\infty} \leq \Lambda_0, \quad \int_0^b h dx = \int_0^b h_0 dx, \right. \\ \left. \int_{\Gamma_{h_{i-1,N}}} \int_0^x (h(\zeta) - h_{i-1,N}(\zeta)) d\zeta d\mathcal{H}^1(x, y) = 0 \right\}.$$

We now show that the incremental minimum problem (36) admits a solution.

Theorem 11. *For every $i = 1, \dots, N$, the minimum problem (36) admits a solution $(\mathbf{u}_{i,N}, h_{i,N}) \in X_{e_0}$.*

Proof. Let $\{(\mathbf{u}_n, h_n)\} \subset X_{e_0}$ be a minimizing sequence for (36). Since $\int_0^b h_n dx = \int_0^b h_0 dx$,

$$\sup_n \int_0^b \frac{(h_n'')^2}{\sqrt{1 + (h_n')^2}} dx < \infty$$

and $\|h_n'\|_{\infty} \leq \Lambda_0$, it follows that $\|h_n\|_{W^{2,2}} \leq C$ for some constant $C > 0$ and for all n . Then, up to a subsequence (not relabelled),

we may assume that $h_n \rightharpoonup h$ weakly in $W_{\#}^{2,2}((0, b); \mathbb{R}^2)$, and thus strongly in $C^1(\mathbb{R}; \mathbb{R}^2)$. As a consequence,

$$\int_{\Gamma_h} \left(\psi(\nu) + \frac{\varepsilon}{2} k^2 \right) d\mathcal{H}^1 \leq \liminf_{n \rightarrow \infty} \int_{\Gamma_{h_n}} \left(\psi(\nu) + \frac{\varepsilon}{2} k_n^2 \right) d\mathcal{H}^1, \quad (38)$$

and

$$\begin{aligned} & \int_{\Gamma_{h_{i-1,N}}} \left(\int_0^x (h(\zeta) - h_{i-1,N}(\zeta)) d\zeta \right)^2 d\mathcal{H}^1 \\ &= \lim_{n \rightarrow \infty} \int_{\Gamma_{h_{i-1,N}}} \left(\int_0^x (h_n(\zeta) - h_{i-1,N}(\zeta)) d\zeta \right)^2 d\mathcal{H}^1. \end{aligned} \quad (39)$$

Finally, since $\sup_n \int_{\Omega_{h_n}} |E(u_n)|^2 dx < \infty$, reasoning as in [20, Proposition 2.2], from the C^1 convergence of $\{h_n\}$ to h and Korn's inequality we deduce that there exists $u \in H_{\text{loc}}^1(\Omega_{\#}^{\#}; \mathbb{R}^2)$ such that $(u, h) \in X_{e_0}$ and, up to a subsequence, $u_n \rightharpoonup u$ weakly in $H_{\text{loc}}^1(\Omega_{\#}^{\#}; \mathbb{R}^2)$. Therefore, we have that

$$\int_{\Omega_h} W(E(u)) dx \leq \liminf_{n \rightarrow \infty} \int_{\Omega_{h_n}} W(E(u_n)) dx,$$

which, together with (38) and (39), allows us to conclude that (u, h) is a minimizer. ■

Next, we show that solutions of the discrete time evolution problems converge to a function $h = h(x, t)$, which is a weak solution of the following geometric evolution equation,

$$\begin{aligned} \frac{\partial h}{\partial t} = & \left[\frac{1}{J} \left(\varepsilon \left(\frac{h_{xx}}{J^5} \right)_{xx} + \frac{5\varepsilon}{2} \left(\frac{h_{xx}^2}{J^7} h_x \right)_x \right. \right. \\ & \left. \left. + (\psi_x(-h_x, 1))_x + W(E(u)) \right) \right]_{x \rightarrow x} \end{aligned} \quad (40)$$

for a short time interval $[0, T_0]$, where $0 < T_0 \leq T$, where T_0 depends on (u_0, h_0) . Here $J := \sqrt{1 + (h_x)^2}$. Since $\|h'_0\|_{\infty} < \Lambda_0$, for all t sufficiently small we have that $\|\frac{\partial h}{\partial t}\|_{\infty} < \Lambda_0$, and so we are allowed to take admissible variations of h to obtain (40).

Theorem 12. *There exist $T_0 \in (0, T]$ and $C > 0$ depending only (h_0, u_0) such that:*

- (i) $h_N \rightarrow h$ in $C^{0,\beta}([0, T_0]; C^{1,\alpha}([0, b]))$ for every $\alpha \in (0, \frac{1}{2})$, and $\beta \in (0, (1 - 2\alpha)/32)$,
- (ii) $E(u_N(\cdot, h_N)) \rightarrow E(u(\cdot, h))$ in $C^{0,\beta}([0, T_0]; C^{1,\alpha}([0, b]))$ for every $\alpha \in (0, \frac{1}{2})$, and $0 \leq \beta < (1 - 2\alpha)/32$, where $u(\cdot, t)$ is the elastic equilibrium in $\Omega_{h(\cdot, t)}$,

and h is a weak solution to (40) with initial data h_0 . Moreover, if $\psi \in C^3(\mathbb{R}^2 \setminus \{0\})$ then $h(\cdot, t) \in H_{\#}^5(0, b)$ for almost every $t \in [0, T_0]$, and h is the unique solution.

For linearly isotropic energy densities of the form (30), where λ and μ satisfy (31), and for sufficiently regular surface energy

densities, we can prove asymptotic stability of the flat configuration $h_{\text{flat}} \equiv d/b$ when d is sufficiently small. Consider the *Grinfeld function* K defined by

$$K(y) := \max_{n \in \mathbb{N}} \frac{1}{n} J(ny), \quad y \geq 0, \quad (41)$$

where

$$J(y) := \frac{y + (3 - 4\nu_p) \sinh y \cosh y}{4(1 - \nu_p)^2 + y^2 + (3 - 4\nu_p) \sinh^2 y},$$

and ν_p is the *Poisson modulus* of the elastic material, i.e.,

$$\nu_p := \frac{\lambda}{2(\lambda + \mu)}. \quad (42)$$

It turns out that K is strictly increasing and continuous, $K(y) \leq Cy$, and $\lim_{y \rightarrow +\infty} K(y) = 1$, for some positive constant C .

Theorem 13. *Assume that W takes the form (30), where λ and μ satisfy (31), and that $\psi \in C^3(\mathbb{R}^2 \setminus \{0\})$ satisfies $\partial_{11}^2 \psi(0, 1) > 0$ and*

$$D^2\psi(\xi)[\tau, \tau] > 0 \quad \text{for all } \tau \perp \xi, \tau \neq 0$$

for every $\xi \in S^1$. Let $d_{\text{loc}} : (0, \infty) \rightarrow (0, \infty]$ be defined as $d_{\text{loc}}(b) := \infty$ if $0 < b \leq \frac{\pi}{4} \frac{(2\mu + \lambda) \partial_{11}^2 \psi(0, 1)}{e_0^2 \mu(\mu + \lambda)}$, and as the solution to

$$K\left(\frac{2\pi d_{\text{loc}}(b)}{b}\right) = \frac{\pi}{4} \frac{(2\mu + \lambda) \partial_{11}^2 \psi(0, 1)}{e_0^2 \mu(\mu + \lambda)} \frac{1}{b} \quad (43)$$

otherwise. Then, for all $d \in (0, d_{\text{loc}}(b))$ the flat configuration $h_{\text{flat}} \equiv d/b$ is asymptotically stable, that is, there exists $\delta > 0$ such that if $h_0 \in W_{\#}^{2,2}((0, b); \mathbb{R}^2)$ with $\int_0^b h_0 dx = d$ and $\|h_0 - h_{\text{flat}}\|_{W^{2,2}} \leq \delta$, then the solution h to (40) with initial datum h_0 exists for all times and

$$\|h(\cdot, t) - h_{\text{flat}}\|_{W^{2,2}} \rightarrow 0$$

as $t \rightarrow \infty$.

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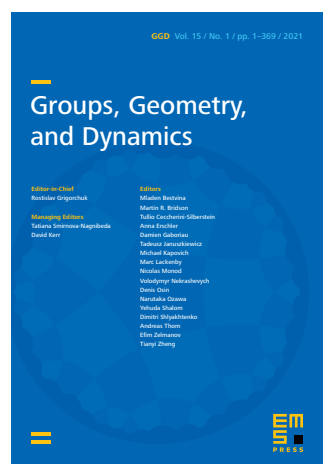
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