Rend. Lincei Mat. Appl. 21 (2010), 341–348
DOI 10.4171/RLM/576

Calculus of Variations — *Equilibrium configurations of epitaxially strained thin films*, by Nicola Fusco, presented on 26 April 2010 by Carlo Sbordone.

To the memory of Renato Caccioppoli, an outstanding mathematician, a great example of civic and moral commitment

Abstract. — We present some regularity results on equilibrium configurations for a variational model introduced to describe the epitaxial growth of an elastic film over a thick flat substrate when a lattice mismatch between the two materials is present. We also give a sufficient condition for local minimality based on second variation and apply it to determine analitycally the critical threshold for the local minimality of the flat configuration.

Key words: Free boundary problems, regularity, local minimality, second variation.

AMS Subject Classification: 74G55, 49K10.

1. The energy functional

We present some recent results on the equilibrium configurations of a free boundary problem introduced by Spencer and Tersoff ([8]) to describe the epitaxial growth of a thin film on a thick rigid substrate. In their model only three-dimensional morphologies with a planar symmetry are considered, thus leading to a two-dimensional problem. The region occupied by the film is denoted by

$$\Omega_h = \{z = (x, y) \in \mathbb{R}^2 : 0 < x < b, 0 < y < h(x)\},$$

where $h : [0, b] \to [0, \infty)$ and its graph Γ_h represents the profile of the film. Denoting by $u : \Omega_h \to \mathbb{R}^2$ the planar displacement of the film and by

$$E(u) = \frac{1}{2}(\nabla u + \nabla^T u)$$

the symmetric part of the gradient of u, the energy associated to a smooth configuration (h, u) is given by

$$G(h, u) = \int_{\Omega_h} \left[\mu|E(u)|^2 + \frac{\lambda}{2}(\operatorname{div} u)^2\right] dz + \sigma_f \mathscr{H}^1(\Gamma_h),$$

where μ and λ are the *Lamé coefficients* of the film, σ_f is a positive constant depending on the surface tension acting on the profile, which up to a rescaling we may assume to be equal to 1, and $\mathcal{H}^1$ denotes the one-dimensional Hausdorff measure.

In order to find equilibrium configurations one tries to minimize G among all configurations (h,u) such that $h(0) = h(b)$, $u(x,0) = e_0(x,0)$ for $0 < x < b$, $e_0 > 0$, $u(b,y) = u(0,y) + e_0(b,0)$ for $0 < y < h(0)$, satisfying the volume constraint $|\Omega_h| = d > 0$.

However, a minimizing sequence for this problem may converge just to a lower semicontinuous function with bounded variation h. Thus the limit profile, beside vertical jumps, may contain also 'cuts' corresponding to points x where $h(x)$ is strictly less than the left and right limits $h(x-)$ e $h(x+)$.

Denote by X the class of all limits of sequences of smooth configurations (h_n, u_n) whose energies are equibounded. Then one can prove (see [1]) that this class consists precisely of all configurations such that $h : \mathbb{R} \to [0,\infty)$ is a lower semicontinuous, b-periodic function with bounded variation in $(0,b)$, and $u \in H^1(\Omega_h;\mathbb{R}^2)$ satisfies the Dirichlet condition $u(x,0) = e_0(x,0)$ and the periodicity condition $u(b,y) = u(0,y) + e_0(b,0)$.

Thus, one may define the energy of a configuration in X by a standard 'relaxation' procedure. It was proved by Bonnetier and Chambolle in [1] (see also [3] for a slightly different model) that the relaxed energy associated to each pair $(h,u) \in X$ is given by

$$F(h,u) = \int_{\Omega_h} \left[\mu|E(u)|^2 + \frac{\lambda}{2}(\operatorname{div} u)^2 \right] dz + \mathcal{H}^1(\Gamma_h) + 2\mathcal{H}^1(\Sigma_h),$$

where $h^-(x) = \min\{h(x-), h(x+)\}$, $h^+(x) = \max\{h(x-), h(x+)\}$, and

$$\Gamma_h = \{(x,y) : 0 \le x < b, h^-(x) \le y \le h^+(x)\},$$
$$\Sigma_h = \{(x,y) : 0 \le x < b, h(x) \le y < h^-(x)\}.$$

Notice that due to the approximation with smooth functions the *vertical cuts* are counted twice in the above representation formula.

As a consequence we have the following existence result.

Theorem 1. *The constrained minimum problem*

$$\min\{F(g,v) : (g,v) \in X, |\Omega_g| = d\} \tag{1}$$

has a solution for all $d > 0$.

2. Regularity of equilibrium configurations

We now discuss the regularity properties of local and global minimizers of the constrained problem (1). By a *local minimizer* for F we mean an admissible configuration $(h,u) \in X$ such that

$$F(h,u) < F(g,v) \tag{2}$$

for every configuration $(g, v) \in X$ such that $0 < d_H(\Gamma_h \cup \Sigma_h, \Gamma_g \cup \Sigma_g) < \delta$ for some $\delta > 0$ and $|\Omega_g| = |\Omega_h|$.

Recall that if A, B are any two sets in $\mathbb{R}^2$ their Hausdorff distance is defined by setting $d_H(A, B) = \inf\{\varepsilon > 0 : B \subset \mathcal{N}_\varepsilon(A) \text{ and } A \subset \mathcal{N}_\varepsilon(B)\}$, where $\mathcal{N}_\varepsilon(A)$ denotes the ε-neighborhood of A. Notice that the use of d_H to measure the distance between the two profiles is due to the presence of vertical cuts. The latter would not be seen by other possible distances like the L^1 or the L^∞ norm of $h - g$. Notice also that if h is continuous, requiring that $d_H(\Gamma_h \cup \Sigma_h, \Gamma_g \cup \Sigma_g)$ is small is equivalent to require that $\sup\{|h(x) - g(x)| : 0 \le x \le b\}$ is small.

A sufficiently smooth local minimizer $(h, u) \in X$ satisfies the following set of Euler–Lagrange equations:

$$(3) \qquad \begin{cases} \mu\Delta u + (\lambda + \mu)\nabla(\operatorname{div} u) = 0 & \text{in } \Omega_h, \\ \sigma(u)[v] = 0 & \text{on } \Gamma_h \cap \{y > 0\}, \\ \sigma(0, y)[v] = -\sigma(b, y)[v] & \text{for } 0 < y < h(0) = h(b), \\ k + \mu|E(u)|^2 + \frac{\lambda}{2}(\operatorname{div} u)^2 = \text{const} & \text{on } \Gamma_h \cap \{y > 0\}, \end{cases}$$

where $\sigma(u) = \mu(\nabla u + \nabla^T u) + \lambda I \operatorname{div} u$, v is the exterior normal to Ω_h and k is the curvature of Γ_h.

Before stating the regularity result proved in [3] we need one more definition. We say that Γ_h has an *inward cups* at $(x, h^-(x))$, $x \in [0, b)$, if $h^-(x) = h(x)$ and $h'(x+) = -h'(x-) = +\infty$. The set of cusp points is denoted by $\Sigma_{h,c}$.

THEOREM 2 (Regularity of local minimizers). *Let $(h, u) \in X$ be a local minimizer for F. Then,*

(i) *there are at most finitely many cusp points and vertical cuts in Γ_h, i.e.,*

$$\operatorname{card}(\{x \in [0, b) : (x, y) \in \Sigma_h \cup \Sigma_{h,c} \textit{ for some } y \ge 0\}) < +\infty;$$

(ii) $\Gamma_h \setminus (\Sigma_h \cup \Sigma_{h,c})$ *is the union of finitely many C^1 arcs;*
(iii) $\Gamma_h \setminus (\Sigma_h \cup \Sigma_{h,c}) \cap \{(x, y) : y > 0\}$ *is of class $C^{1,\alpha}$ for all $\alpha \in (0, 1/2)$;*
(iv) *let $A := \{x \in \mathbb{R} : h(x) > 0$ and his continuous at $x\}$. Then A is an open set, dense in $\{h > 0\}$, and h is analytic in A.*

Statement (ii) in Theorem 2 implies in particular the *zero contact angle condition* at the interface between film and substrate, i.e., $h'(x) = 0$ for all $x \in [0, b)$ such that $(x, 0) \notin \Sigma_h \cup \Sigma_{h,c}$.

Notice also that if $h > 0$, Γ_h is of class $C^{1,\alpha}$ for some $\alpha \in (0, 1)$, and $(h, u) \in X$ satisfies the first three equations in (3), standard elliptic regularity implies (see e.g. [4, Proposition 8.9]) that $u \in C^{1,\alpha}(\overline{\Omega}_h)$. Moreover, if also $(3)_4$ holds, the results proved in [7, Sez. 4.2] yield that h is analytic.

Finally, we point out that in [3] a slightly different model and a slightly stronger notion of local minimality are considered. However, the regularity results proved therein do apply also to the model discussed here.

The proof of Theorem 2 is rather long. Here, we just sketch the main steps and ideas. All details can be found in [3].

The first step toward regularity is to remove the constraint $|\Omega_h| = d$ by showing that if (h, u) is a local minimizer, then (h, u) is also a local minimizer of the penalized functional

$$(g, v) \in X \mapsto F(g, v) + \Lambda| \, |\Omega_g| - d|,$$

for some sufficiently large $\Lambda > 0$. This allows us to use a wider range of variations thus showing that $\Omega_h^{\#}$, the set obtained by b-periodic extension of Ω_h in the horizontal direction, satisfies a uniform interior ball condition. To be precise, one proves that given a sufficiently small $\varrho > 0$, for all $z_0 \in \partial\Omega_h^{\#}$ there exists an open disk $B_\varrho(z) \subset \Omega_h^{\#}$ such that $\partial B_\varrho(z) \cap \partial\Omega_h^{\#} = \{z_0\}$.

In fact, assume that the boundary of the disk $B_\varrho(z) \subset \Omega_h^{\#}$ intersects $\partial\Omega_h^{\#}$ at two points (x_1, y_1), (x_2, y_2). To fix the ideas, take $0 \le x_1 < x_2 < b$. Then, denote by $\tilde{h}$ the function coinciding with h in $[0, b)\backslash[x_1, x_2]$ and defined in (x_1, x_2) as the function whose graph is the segment with endpoints (x_1, y_1) e (x_2, y_2). Notice that if (h, u) satisfies the local minimality condition (2) for some $\delta > 0$, then there exists $\varrho_0 > 0$ such that $d_H(\Gamma_h \cup \Sigma_h, \Gamma_{\tilde{h}} \cup \Sigma_{\tilde{h}}) < \delta$ for all $\varrho \in (0, \varrho_0)$. A comparison of the energies yields

$$[F(h, u) + \Lambda| \, |\Omega_h| - d|] - [F(\tilde{h}, u) + \Lambda| \, |\Omega_{\tilde{h}}| - d|] \ge (L - \ell) - \Lambda|D|,$$

where ℓ is the length of the segment from (x_1, y_1) to (x_2, y_2), L is the length of the subarc of Γ_h connecting these two points and D is the region bounded by the two curves. From the isoperimetric inequality

$$L - \ell \ge \frac{\kappa}{\varrho}|D|,$$

where $\kappa > 0$ is a universal constant, we conclude, by the minimality of u, that ϱ must be necessarily larger than or equal to κ/Λ.

The uniform interior ball condition implies in turn that $\partial\Omega_h^{\#}$ has (locally) finitely many cuts and cusps. Moreover, outside these singular points $\partial\Omega_h^{\#}$ is the union of (locally) finitely many graphs of Lipschitz functions having left and right derivatives at every point which are left and right continuous, respectively (see [2]).

To show that there are no corner points away from the singular points, thus proving that $\Gamma_h\backslash(\Sigma_h \cup \Sigma_{h,c})$ is a C^1 manifold, we argue by contradiction. In fact, if Γ_h had a corner at $z_0 = (x_0, y_0)$, the classical estimates by Grisvard ([6]) on the singularities of solutions to linear systems of elasticity in domains with corners, combined with a blow-up argument, would imply that there exist $r_0, C_0 > 0$ such that for all $0 < r \le r_0$

$$\int_{B_r(z_0)\cap\Omega_h} |Du|^2 \, dz \le C_0 r^{2\beta},$$

for some $\beta > 1/2$. Given this estimate, one could extend u to the whole disk $B_{r_0}(z_0)$ in such a way that the resulting function $\tilde{u}$ satisfies for all $0 < r \le r_0$

$$\int_{B_r(z_0)} |D\tilde{u}|^2 \, dz \le C_1 r^{2\beta}, \tag{4}$$

with C_1 not depending on r. Thus, given a sufficiently small r, let (x_1, y_1), $(x_2, y_2) \in \partial\Omega_h^{\#} \cap \partial B_r(z_0)$ be two points such that $x_1 < x_0 < x_2$ and $\partial\Omega_h^{\#} \cap ((x_1, x_2) \times \mathbb{R}) \subset B_r(z_0)$. Defining $\tilde{h}$ as before and comparing the energies at the two configurations (h, u), $(\tilde{h}, \tilde{u})$, one easily gets from (4) and from the fact that $\beta > 1/2$,

$$[F(h,u) + \Lambda| \, |\Omega_h| - d|] - [F(\tilde{h}, \tilde{u}) + \Lambda| \, |\Omega_{\tilde{h}}| - d|] \ge 2r(1 - \sin(\vartheta_0/2)) + o(r),$$

where ϑ_0 is the angle formed by the left and right tangents at z_0. Thus, the local minimality of (h, u) implies that $\vartheta_0 = \pi$ and z_0 is not a corner point.

The proof of statement (iii) of Theorem 2 combines in similar way elliptic regularity results and variational arguments, while (iv) follows from the general results proved in [7].

3. Second variation and minimality

We now come to the qualitative properties of equilibrium configurations. The results we present here are proved in [4]. A first problem discussed in that paper is to determine sufficient conditions for the local minimality of an admissible configuration, based on a suitable notion of second variation for F.

To this aim, given a pair $(h, u) \in X$, with $h \in C^2([0, b])$, we say that (h, u) is a *critical point* for F if it satisfies the system of Euler–Lagrange equations (3). Notice that the *flat configuration* of volume d

$$h \equiv \frac{d}{b}, \quad u_0(x, y) := e_0\left(x, \frac{-\lambda}{2\mu + \lambda} y\right),$$

is always a critical point.

Let us now introduce the notion of second variation of F for a configuration $(h, u) \in X$, with $h \in C^\infty([0, b])$, $h > 0$, where u is the corresponding elastic equilibrium, i.e., the minimum of the elastic energy in Ω_h, under the periodicity and boundary conditions indicated in the previous section.

Given a variation $\varphi \in H^1(0, b)$, $\varphi(0) = \varphi(b)$, with $\int_0^b \varphi \, dx = 0$, we set for $|t|$ small enough $h_t := h + t\varphi$ and denote by u_t the corresponding elastic equilibrium. Notice that $(h_t, u_t) \in X$ and that $|\Omega_h| = |\Omega_{h_t}|$. Then, the second variation of F at (h, u) along the direction φ is defined as

$$\partial^2 F(h, u)[\varphi] := \frac{d^2}{dt^2} F(h_t, u_t)_{|t=0}.$$

We say that the second variation at (h,u) is *positive definite* if $\partial^2 F(h,u)[\varphi] > 0$ for all $\varphi \neq 0$.

THEOREM 3. *Let $(h,u) \in X$ be a critical point for F, with $h \in C^\infty([0,b])$ and $h > 0$, such that the second variation of F is positive definite at (h,u). Then (h,u) is a local minimizer.*

To the best of our knowledge this result is the first local minimality criterion based on the second variation for a free boundary problem. Indeed, we think that many of the ideas used in [4] can be used to deal with similar variational problems.

The representation formula for the second variation of F has a rather complicate expression (see [4, Theorem 3.2]), which simplifies a lot in the case of flat configuration. In fact, given $d > 0$, one has that for every $\varphi \in H^1(0,b)$, $\varphi(0) = \varphi(b)$, with $\int_0^b \varphi\, dx = 0$,

$$\partial^2 F(d/b, u_0)[\varphi] = -2\int_R Q(E(v_\varphi))\, dz + \int_0^b \varphi'^2\, dx,$$

where $R = (0,b) \times (0, d/b)$ and v_φ is the solution of the system

$$\begin{cases} (2\mu+\lambda)\dfrac{\partial^2 v_\varphi^1}{\partial x^2} + \mu\dfrac{\partial^2 v_\varphi^1}{\partial y^2} + (\lambda+\mu)\dfrac{\partial^2 v_\varphi^2}{\partial x \partial y} = 0 & \text{in } R, \\ \mu\dfrac{\partial^2 v_\varphi^2}{\partial x^2} + (2\mu+\lambda)\dfrac{\partial^2 v_\varphi^2}{\partial y^2} + (\lambda+\mu)\dfrac{\partial^2 v_\varphi^1}{\partial x \partial y} = 0 & \text{in } R, \end{cases}$$

satisfying the periodicity condition $v_\varphi(b,y) = v_\varphi(0,y) + e_0(b,0)$ and the boundary conditions

$$\begin{cases} \dfrac{\partial v_\varphi^1}{\partial y} + \dfrac{\partial v_\varphi^2}{\partial x} = \dfrac{4(\mu+\lambda)e_0}{2\mu+\lambda}\varphi',\ \lambda\dfrac{\partial v_\varphi^1}{\partial x} + (2\mu+\lambda)\dfrac{\partial v_\varphi^2}{\partial y} = 0 & \text{on } \{y = d/b\}, \\ v_\varphi = 0 & \text{on } \{y = 0\}. \end{cases}$$

The solution v_φ can be explicitely determined by Fourier series expansion (see [5] and [4]), thus obtaining an explicit formula for $\partial^2 F(d/b, u_{e_0})$. To this aim, we set

$$v_p := \frac{\lambda}{2(\lambda+\mu)}, \qquad \tau := e_0 \frac{4\mu(\mu+\lambda)}{2\mu+\lambda}$$

and introduce the function $J : (0,\infty) \to (0,\infty)$ defined as

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

The quantity v_p is known as the *Poisson modulus* of the elastic material.

PROPOSITION 4. *Given $d > 0$, for any $\varphi \in H^1(0,b)$, $\varphi(0) = \varphi(b)$, with $\int_0^b \varphi = 0$, we have*

$$\partial^2 F(d/b, u_{e_0})[\varphi] = \sum_{n\in\mathbb{Z}} n^2 \varphi_n \varphi_{-n} \left[1 - \frac{\tau^2(1-\nu_p)bJ(2\pi nd/b^2)}{2\pi\mu n}\right],$$

where the φ_n's are the Fourier coefficients of φ in the interval $(0,b)$.

By combining the minimality criterion stated in Theorem 3 with the explicit formula provided by the previous proposition, we immediately get the necessary and sufficient conditions for the local minimality of the flat configuration contained in Theorem 5 below. But first we need to introduce the *Grinfeld function* K defined for $y \geq 0$ as

$$K(y) := \max_{n\in\mathbb{N}} \frac{1}{n} J(ny).$$

It can be shown ([4, Corollary 5.3]) that

$$K \text{ is strictly increasing and continuous, } K(y) \leq Cy \text{ and } \lim_{y\to+\infty} K(y) = 1,$$

for a suitable constant C.

THEOREM 5. *Let $d_{\mathrm{loc}} : (0,+\infty) \to (0,+\infty]$ be defined as $d_{\mathrm{loc}}(b) := +\infty$, if $0 < b \leq \frac{\pi}{4}\frac{2\mu+\lambda}{e_0^2\mu(\mu+\lambda)}$, and as the unique solution of the equation*

$$K\left(\frac{2\pi d_{\mathrm{loc}}(b)}{b^2}\right) = \frac{\pi}{4}\frac{2\mu+\lambda}{e_0^2\mu(\mu+\lambda)}\frac{1}{b},$$

otherwise. Then, the flat configuration $(d/b, u_0)$ is a local minimizer for F whenever $0 < d < d_{\mathrm{loc}}(b)$.

The value d_{loc} is a critical threshold: in fact, if $d > d_{\mathrm{loc}}(b)$, there exists $(g,v) \in X$, with $|\Omega_g| = d$ and $d_H(\Gamma_{d/b}, \Gamma_g \cup \Sigma_g)$ arbitrarily small, such that $F(g,v) < F(d/b, u_0)$.

Notice that if $0 < b \leq \frac{\pi}{4}\frac{2\mu+\lambda}{e_0^2\mu(\mu+\lambda)}$ then the above theorem implies that the flat configuration is always a local minimizer.

While Theorem 5 gives the precise threshold for the local minimality of the flat configuration, next result is more qualitative but deals with the stronger notion of global minimality. Together with other qualitative properties of non flat minimizers also this result is proved in [4].

THEOREM 6. *For the flat configuration $(d/b, u_0)$ the two follwing properties hold.*

(i) *For every $b > 0$, there exists $0 < d_{\mathrm{glob}}(b) \leq d_{\mathrm{loc}}(b)$ (see Theorem 5) such that $(d/b, u_0)$ is a global minimizer if and only if $0 < d \leq d_{\mathrm{glob}}(b)$. Moreover, if $0 < d < d_{\mathrm{glob}}(b)$, then $(d/b, u_0)$ is the unique global minimizer.*

(ii) *There exists* $0 < b_{\mathrm{crit}} \le \frac{\pi}{4}\frac{2\mu+\lambda}{e_0^2\mu(\mu+\lambda)}$ *such that* $d_{\mathrm{glob}}(b) = +\infty$ *if and only if* $0 < b \le b_{\mathrm{crit}}$, *i.e., the flat configuration* $(d/b, u_0)$ *is the unique global minimizer for all* $d > 0$ *if and only if* $0 < b \le b_{\mathrm{crit}}$.

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Received 12 April 2010,
and in revised form 26 April 2010.

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