Regularity and optimality conditions for a free boundary problem
Part I (Preliminary Version)

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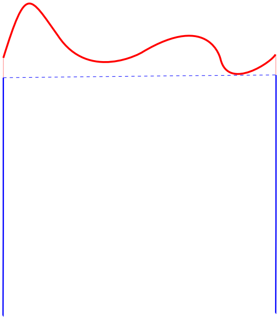

I.Fonseca,N.F., G.Leoni, M.Morini (2007)
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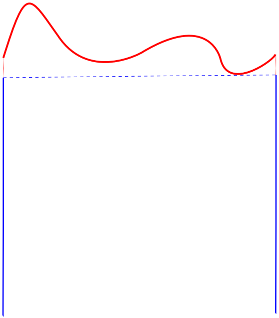
Deposition of a thin film on a thick substrate

Mismatch strain

$\Downarrow$

formation of 'islands'



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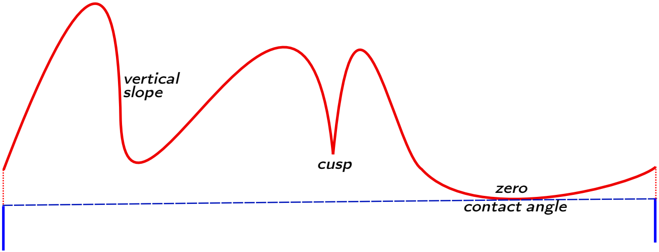


Three dimensional configurations with planar symmetries

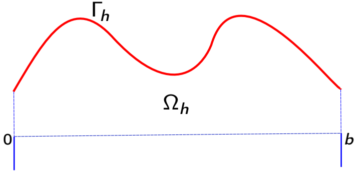
$\Downarrow$

2-D Model

B.Spencer, D.Meiron (Acta Metal. Mater., 1994)
B.Spencer, J.Tersoff (Phy. Rev. Letter, 1997)

Numerical results: C.Chiu, H.Gao
R.Nochetto, M.Paolini, S.Rovida, C.Verdi

Analysis: M.Grinfeld
S.Nicaise
E.Bonnetier, A.Chambolle (2002)

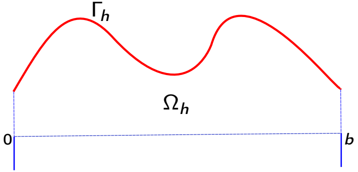


$h : \mathbb{R} \to [0, \infty)$ b-periodic, smooth

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

$\Gamma_h := \partial\Omega_h \cap \{y > 0\}$

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



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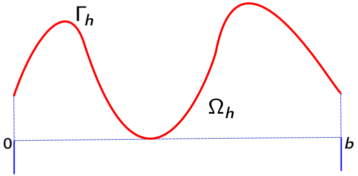
Γ_h = free profile of the film

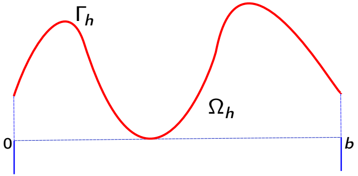
Ω_h = final configuration of the film, $|\Omega_h| = d$ is given

$u : \Omega_h \mapsto \mathbb{R}^2$ = planar displacement of the film



$u(x,0) = e_0(x,0)$
at the film-substrate interface
($e_0 \neq 0$ is the mismatch factor)

$u(b,y) = u(0,y) + e_0(b,0)$
if $0 \leq y \leq h(0) = h(b)$



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Moreover

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

$W(E) := \mu|E|^2 + \frac{\lambda}{2}\big[Tr(E)\big]^2 = \frac{1}{2}\mathbb{C}E : E =$ elastic energy per volume unit

$\mu > 0, \ \lambda + \mu > 0, \qquad \mu, \lambda$ are the Lamé constants

$$\mathbb{C}E := \begin{pmatrix} (2\mu + \lambda)E_{11} + \lambda E_{22} & 2\mu E_{12} \\ 2\mu E_{12} & (2\mu + \lambda)E_{22} + \lambda E_{11} \end{pmatrix}$$

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Since

$$W(E) \geq \min\{\mu, \mu+\lambda\}|E|^2 \qquad \text{for all } E \in \mathbb{M}^{2\times 2}_{\mathrm{sym}},$$

conditions $\mu > 0, \ \lambda + \mu > 0$ guarantee that W is coercive.

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For a smooth profile the total energy is:

$$G(h, u) = \int_{\Omega_h} W\big(E(u)\big)\,dz + \gamma_f \mathcal{H}^1(\Gamma_h)$$

where $\gamma_f > 0$

$$\inf\Big\{ G(h,u) : \ h \text{ is } b\text{-periodic and smooth}, \ |\Omega_h| = d, \\ u \in H^1_{loc}(\Omega_h, \mathbb{R}^2) + \text{Dirichlet \& period. cond.} \Big\}$$

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If (h,u) is a smooth minimizer then

$$(LS) \qquad \begin{cases} \mu\Delta u + (\lambda+\mu)\nabla(div\, u) = 0 & \text{in } \Omega_h \\ \qquad\qquad + & \\ \big[\mu(\nabla u + \nabla^T u) + \lambda(div\, u) Id\big]\nu = 0 & \text{on } \Gamma_h \\ u(x,0) = e_0(x,0) & \text{on } \{y=0\} \\ u(b,y) = u(0,y) + e_0(b,0) & 0 \le y \le h(0) \end{cases}$$

and

$$(CE) \qquad \frac{d}{dx}\Big(\frac{h'}{\sqrt{1+h'^2}}\Big) = W\big(E(u)\big)(x,h(x)) + const.$$

No minimizer $\Longrightarrow$ Relaxation procedure

Remark: if $\sup_n G(h_n, u_n) < \infty$, we have

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$$\sup_n \int_0^b \sqrt{1 + h_n'^2}\,dx < \infty, \qquad \int_0^b h_n\,dx = d$$

$$\Downarrow$$

$$0 \le h_n(x) \le M$$

and

$$\sup_n \int_{\Omega_{h_n}} |E(u_n)|^2 dz < \infty \qquad u_n(x,0) = e_0(x,0)$$

Therefore, up to a subsequence......

Remark: if $\sup_n G(h_n, u_n) < \infty$, we have

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$$\mathbb{R}^2 \setminus \Omega^{\#}_{h_n} \to \mathbb{R}^2 \setminus \Omega^{\#}_{h} \qquad \text{in the Hausdorff metric } d_H$$

$$u_n \to u \qquad \text{weakly in } H^1_{loc}(\Omega^{\#}_h, \mathbb{R}^2)$$

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Recall that for any pair (A, B) of subsets of $\mathbb{R}^2$

$$d_H(A, B) := \inf\{\varepsilon > 0 : \, B \subset \mathcal{N}_\varepsilon(A) \text{ and } A \subset \mathcal{N}_\varepsilon(B)\},$$

where $\mathcal{N}_\varepsilon(A)$ denotes the ε-neighborhood of A.

The space of all reachable configurations

$$X = \Big\{(h,u): \ h \text{ is l.s.c., } b\text{-periodic}, h \in BV_{loc}(\mathbb{R}),\ u \in H^1_{loc}(\Omega_h^{\#};\mathbb{R}^2),$$
$$u(x,0)=e_0(x,0),\ u(b,y)=u(0,y)+e_0(b,0) \text{ for } 0\le y\le h(0)\Big\}$$

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$$F(h,u) = \inf\{\liminf_n G(h_n,u_n): \ (h_n,u_n) \in X, \ h_n \text{ smooth},$$
$$(h_n,u_n) \to (h,u) \text{ in the sense defined above}\}$$

How can we represent $F(h,u)$?

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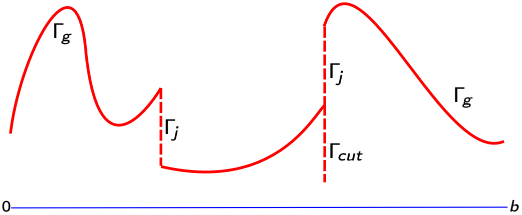
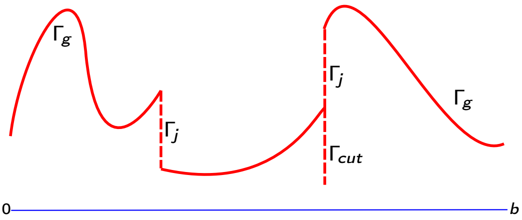
How can we represent $F(h,u)$?

Recall that h is l.s.c. and BV, hence for all x there exist $h(x\pm)$ and

$$h(x) \le h^-(x) := \min\{h(x-), h(x+)\} \le h^+(x) := \min\{h(x-), h(x+)\}$$



$$\Gamma = \Gamma_g \cup \Gamma_j \cup \Gamma_{cut} = \widetilde{\Gamma} \cup \Gamma_{cut}$$



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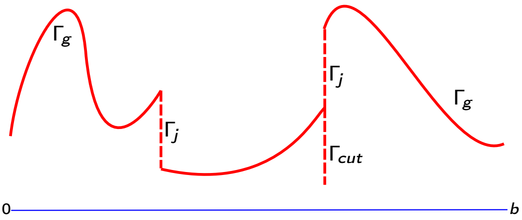
Representation formula (Bonnetier-Chambolle, also FFLM)

$$F(h,u) = \int_{\Omega_h} W\big(E(u)\big)\,dz + \gamma_f \mathcal{H}^1(\widetilde{\Gamma}_h) + 2\gamma_f \mathcal{H}^1(\Gamma_{h,cut})$$



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where

$$\widetilde{\Gamma}_h = \{(x,y) :\ x \in [0,b),\ h^-(x) \le y \le h^+(x)\}$$
$$\Gamma_{h,cut} = \{(x,y) :\ x \in [0,b),\ h(x) \le y \le h^-(x)\}$$

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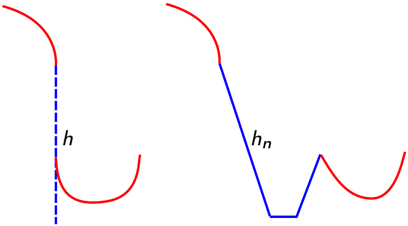

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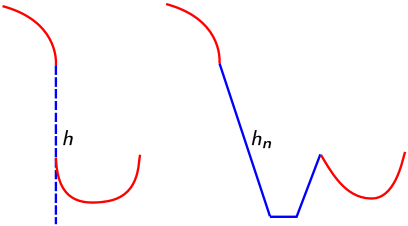

Moreover the minimum problem

$$\inf\Big\{F(h,u): \ (h,u)\in X, \ |\Omega_h| = d\Big\}$$

has at least a solution

Theorem. Regularity (Fonseca, F., Leoni, Morini)

If $(h, u) \in X$ is a minimum configuration for F, under the constraint $|\Omega_h| = d$,

- *there are only finitely many vertical cuts and cusps*
- $\Gamma_{reg} = \Gamma_h \setminus \left(\Gamma_{cut} \cup \Gamma_{cusp}\right)$ *is the union of finitely many C^1-arcs*
- $\Gamma_{reg} \cap \{y > 0\}$ *is of class $C^{1,\alpha}$ for all* $0 < \alpha < \dfrac{1}{2}$
- *h is analytic in the open set* $\{x : \ h(x) > 0, \ h \text{ is continuous}\}$

$$\Gamma_{cusp} := \left\{(x, h(x)) : \ h^-(x) = h^+(x) = h(x), \ h'_+(x) = -h'_-(x) = +\infty\right\}$$
$$= \left\{ \text{downward cusps} \right\}$$

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Remark: the theorem proves the zero contact angle condition

From now on $\gamma_f = 1$. Fix $d = |\Omega_h|$ and denote by

$$\left(\frac{d}{b}, u_0\right) \qquad \text{the flat configuration}$$

where

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

is the minimum of the elastic energy

$$\int_{\Omega_h} W\big(E(u)\big)dz = \int_{\Omega_h}\Big\{\mu|E(u)|^2 + \frac{\lambda}{2}\big[Tr(E(u)\big]^2\Big\}dz$$

under the Dirichlet condition $u(x,0) = e_0(x,0)$ and the periodicity condition.

Set $E_0 := E(u_0) = const.$

Regularity 1: Penalization

If $\Lambda > W(E_0)$, *any minimizer* $(h, u) \in X$ *of* F *under the constraint* $|\Omega_h| = d$ *is also a minimizer of the unconstrained problem*

$$\inf\Big\{F(g, v) + \Lambda\big||\Omega_g| - d\big| : (g, v) \in X\Big\}$$

Proof.

Let (g, v) be a minimizer for the unconstrained problem.
If $|\Omega_g| > d$, just truncate g so that the resulting function $\tilde{g}$ is such that

$$|\Omega_{\tilde{g}}| = d\,.$$

Then $(\tilde{g}, v)$ is a configuration with strictly less energy, since

$$F(\tilde{g}, v) < F(g, v), \qquad 0 = \Lambda\big||\Omega_{\tilde{g}}| - d\big| < \Lambda\big||\Omega_g| - d\big|$$

Proof.

If $|\Omega_g| < d$, lift g setting $\tilde{g} := g + \frac{d - |\Omega_g|}{b}$
and extend v, setting

$$\tilde{v}(x,y) = \begin{cases} e_0\Big(x, \frac{-\lambda}{2\mu+\lambda} y\Big) & \text{if } 0 < y < \frac{d-|\Omega_g|}{b} \\ v\Big(x, y - \frac{d-|\Omega_g|}{b}\Big) + e_0\Big(0, \frac{-\lambda(d-|\Omega_g|)}{b(2\mu+\lambda)}\Big) & \text{if } y \geq \frac{d-|\Omega_g|}{b}\,. \end{cases}$$

Then

$$\begin{aligned} F(\tilde{g},\tilde{v}) + \Lambda\Big||\Omega_{\tilde{g}}| - d\Big| - F(g,v) - \Lambda\Big||\Omega_g| - d\Big| \\ = W(E_0)(d - |\Omega_g|) - \Lambda(d - |\Omega_g|) < 0\,, \end{aligned}$$

which is a contradiction to the minimality of (g,v). $\square$

Regularity 2: Interior ball condition

If $(h,u) \in X$ *is a minimizer in* X *of*

$$F(g,v) + \Lambda \big| |\Omega_g| - d \big|$$

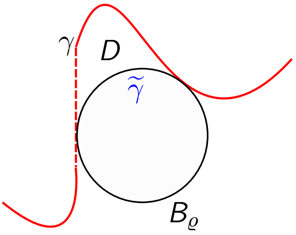
for all $z \in \Gamma_h$ *and* $0 < \varrho < \dfrac{1}{\Lambda}$ *there exists a ball* $B_\varrho \subset \Omega_h$ *such that*

$$\overline{B}_\varrho \cap \Gamma_h = \{z\}$$

Proof.

Since (h, u) minimizes

$$\int_{\Omega_g} W\big(E(v)\big)\,dz + \mathcal{H}^1(\widetilde{\Gamma}_g) + 2\mathcal{H}^1(\Gamma_{g,cut}) + \Lambda\big||\Omega_g| - d\big|$$



If we replace h by $\widetilde{h}$

we gain $\mathcal{H}^1(\gamma) - \mathcal{H}^1(\widetilde{\gamma})$

we pay $\Lambda|D|$

□

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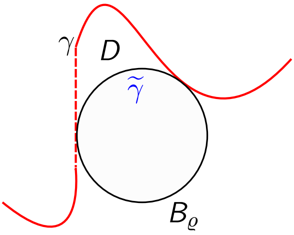


If we replace h by $\widetilde{h}$

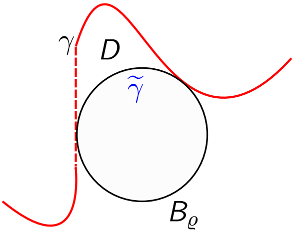
we gain $\mathcal{H}^1(\gamma) - \mathcal{H}^1(\widetilde{\gamma})$

we pay $\Lambda|D|$

But from the 'isoperimetric inequality' we get that

$$\mathcal{H}^1(\gamma) - \mathcal{H}^1(\widetilde{\gamma}) \geq \frac{1}{\varrho}|D| > \Lambda|D| \qquad \text{impossible!!}$$

□



Let $[\alpha, \beta]$ be the projection

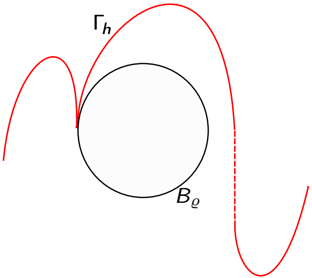
of γ on the x axis

and assume that $h \in C^1([\alpha, \beta])$

Then

$$
\begin{aligned}
\mathcal{H}^1(\gamma) - \mathcal{H}^1(\widetilde{\gamma}) &= \int_\alpha^\beta \sqrt{1 + h'^2} - \int_\alpha^\beta \sqrt{1 + \widetilde{h}'^2} \\
&\geq \int_\alpha^\beta \frac{(h' - \widetilde{h}')\widetilde{h}'}{\sqrt{1 + \widetilde{h}'^2}} \\
&= \int_\alpha^\beta (h - \widetilde{h}) \Big(\frac{-\widetilde{h}'}{\sqrt{1 + \widetilde{h}'^2}} \Big)' \\
&= \frac{1}{\varrho} \int_\alpha^\beta (h - \widetilde{h}) = \frac{1}{\varrho} |D|
\end{aligned}
$$

Regularity 3: Consequences of the interior ball condition



Γ_h has finitely many cut segments and cusps

Moreover if $z_0 \in \Gamma_h \setminus \left(\Gamma_j \cup \Gamma_{cut} \cup \Gamma_{cusp}\right)$ there exists a nhood $I(z_0)$ such that

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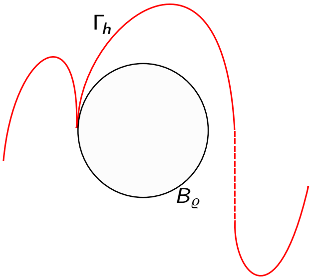

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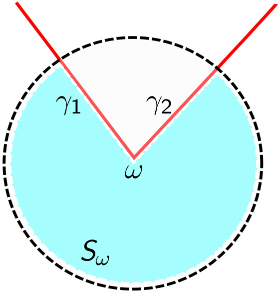
Moreover if $z_0 \in \Gamma_h \setminus \left(\Gamma_j \cup \Gamma_{cut} \cup \Gamma_{cusp}\right)$
there exists a nhood $I(z_0)$ such that

$\Gamma_h \cap I(z_0)$ is the graph of a Lipschitz function,

having right (resp. left) derivatives at every point
that are right (resp. left) continuous

Regularity 4: Grisvard revisited & blow-up



Let S_ω be a sector of the unit disk
with $0 < \omega < \pi$
$w \in H^1(S_\omega; \mathbb{R}^2)$ a weak solution of

$$\mu \Delta w + (\lambda + \mu) \nabla (div\, w) = 0 \quad \text{in } S_\omega$$

such that on $\gamma_1 \cup \gamma_2$

$$\sigma(w)\nu := \left[\mu(\nabla w + \nabla^T w) + \lambda (div\, w) Id\right]\nu = 0$$

Theorem (Grisvard & FFLM)

Let S_ω and w be as above. Then, there exist $1/2 < \beta < 1$ and $C_0 > 0$ such that

$$\int_{B_r \cap S_\omega} |\nabla w|^2 dz \leq C_0 r^{2\beta} \int_{S_\omega} \left(|w|^2 + |\nabla w|^2\right) dz \qquad \forall r < 1$$

Remarks:

- β depends only on ω and $\beta(\omega) \to 1/2$ if $\omega \to 0^+$
- $\beta(\pi) = 1$
- C_0 depends only on ω, μ, λ

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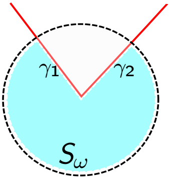

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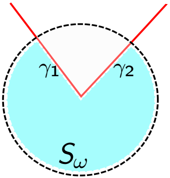

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