Variational Methods for Crystal Surface Instability

Irene Fonseca

Department of Mathematical Sciences
Center for Nonlinear Analysis
Carnegie Mellon University
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Epitaxy: Outline

- Quantum Dots: wetting and zero contact angle. Shapes of islands
- surface diffusion in epitaxially strained solids
- material voids

Quantum Dots. The Context

With N. Fusco, G. Leoni, M. Morini

Strained epitaxial films on a relatively thick substrate; the thin film wets the substrate.
Islands develop without forming dislocations – Stranski-Krastanow growth

plane linear elasticity (In-GaAs/GaAs or SiGe/Si)

- free surface of film is *flat* until reaching a critical thikness
- *lattice misfits* between substrate and film induce *strains* in the film
- Complete relaxation to bulk equilibrium ⇒ crystalline structure would be discontinuous at the interface
- Strain ⇒ flat layer of film morphologically unstable or metastable after a critical value of the thickness is reached (competition between surface and bulk energies)

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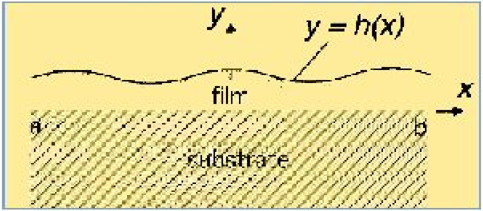
Islands

To release some of the elastic energy due to the strain: atoms on the free surface rearrange and morphologies such as formation of island (*quatum dots*) of pyramidal shapes are energetically more economical

the profile



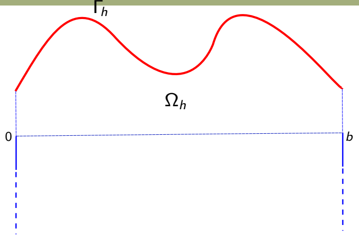
Kinetics of Stranski-Krastanow depend on initial thickness of film, competition between strain and surface energies, anisotropy, ETC.

Quantum Dots: "semiconductors whose characteristics are closely related to size and shape of crystals"

transistors, solar cells, optical and optoelectric devices (quantum dot laser), medical imaging, information storage, nanotechnology . . .

electronic properties depend on the *regularity* of the dots, *size*, *spacing*, etc.

Sharp Interface Model



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

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

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

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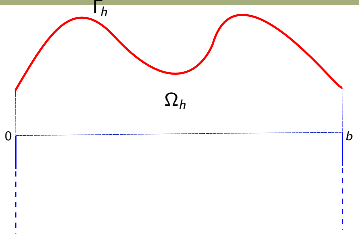

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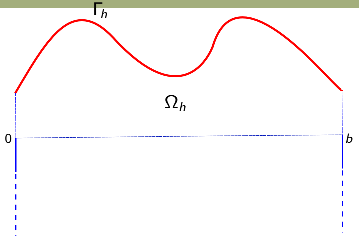

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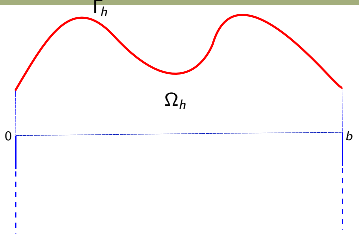

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- $u : \Omega_h \mapsto \mathbb{R}^2$ = displacement of the film

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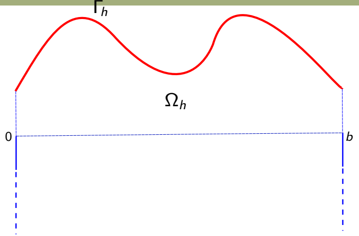

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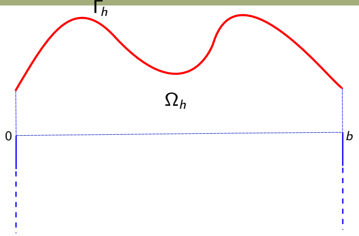

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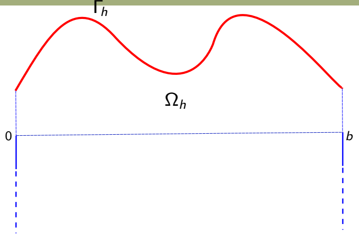

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Brian Spencer, Bonnetier and Chambolle, Chambolle and Larsen; Caflish, W. E, Otto, Voorhees, et. al.

epitaxial thin films: Gao and Nix, Spencer and Meiron, Spencer and Tersoff, Chambolle, Braides, Bonnetier, Solci, F., Fusco, Leoni, Morini

anisotropic surface energies: Herring, Taylor, Ambrosio, Novaga, and Paolini, Fonseca and Müller, Morgan *mismatch strain* (at which minimum energy is attained)

$$\mathbf{E}_0(y) = \begin{cases} e_0 \mathbf{i} \otimes \mathbf{i} & \text{if } y \geq 0, \\ 0 & \text{if } y < 0, \end{cases}$$

$e_0 > 0$

$\mathbf{i}$ the unit vector along the x direction

elastic energy per unit area: $W(\mathbf{E} - \mathbf{E}_0(y))$

$$W(\mathbf{E}) := \frac{1}{2}\mathbf{E} \cdot \mathbb{C}[\mathbf{E}], \quad \mathbf{E}(u) := \frac{1}{2}(\nabla u + (\nabla u)^T)$$

$\mathbb{C}$ . . . positive definite fourth-order tensor

film and substrate have similar material properties, share the same homogeneous elasticity tensor $\mathbb{C}$

$$\varphi_0(y) := \begin{cases} \gamma_{\text{film}} & \text{if } y > 0, \\ \gamma_{\text{sub}} & \text{if } y = 0. \end{cases}$$

Total energy of the system:

$$F(\mathbf{u}, \Omega_h) := \int_{\Omega_h} W(\mathbf{E}(\mathbf{u})(\mathbf{x}) - \mathbf{E}_0(y))\, d\mathbf{x} + \int_{\Gamma_h} \varphi_0(y)\, d\mathcal{H}^1(\mathbf{x}),$$

$\Gamma_h := \partial\Omega_h \cap ((0, b) \times \mathbb{R})$ ... *free surface of the film*

Hard to Implement ...

Sharp interface model is difficult to be implemented numerically. Instead: *boundary-layer model*; discontinuous transition is regularized over a thin transition region of width δ ("smearing parameter").

$$\mathbf{E}_\delta(y) := \frac{1}{2} e_0 \left(1 + f\left(\frac{y}{\delta}\right)\right) \mathbf{i} \otimes \mathbf{i}, \quad y \in \mathbb{R},$$

$$\varphi_\delta(y) := \gamma_{\text{sub}} + (\gamma_{\text{film}} - \gamma_{\text{sub}}) f\left(\frac{y}{\delta}\right), \quad y \geq 0,$$

$$f(0) = 0, \quad \lim_{y \to -\infty} f(y) = -1, \quad \lim_{y \to \infty} f(y) = 1.$$

Regularized total energy of the system

$$F_\delta(\mathbf{u},\Omega_h) := \int_{\Omega_h} W\left(\mathbf{E}(\mathbf{u})(\mathbf{x}) - \mathbf{E}_\delta(y)\right)\, d\mathbf{x} + \int_{\Gamma_h} \varphi_\delta(y)\, d\mathcal{H}^1(\mathbf{x})$$

$$\text{Two regimes}: \begin{cases} \gamma_{\text{film}} \geq \gamma_{\text{sub}} \\ \gamma_{\text{film}} < \gamma_{\text{sub}} \end{cases}$$

Wetting, etc.

asymptotics as $\delta \to 0^+$

- $\gamma_{\text{film}} < \gamma_{\text{sub}}$
  relaxed surface energy density is no longer discontinuous: it is constantly equal to γ_{film}... WETTING!
- more favorable to cover the substrate with an infinitesimal layer of film atoms (and pay surface energy with density γ_{film}) rather than to leave any part of the substrate exposed (and pay surface energy with density γ_{sub})
- wetting regime: regularity of local minimizers $(\mathbf{u}, \Omega)$ of the limiting functional F_∞ under a volume constraint.

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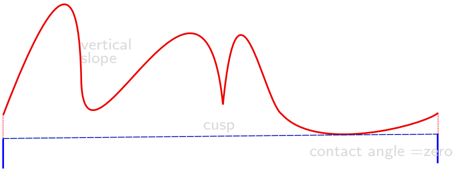
cusps and vertical cuts

The profile *h* of the film for a locally minimizing configuration is regular except for at most a finite number of *cusps* and *vertical cuts* which correspond to vertical cracks in the film.

[Spencer and Meiron]: steady state solutions exhibit cusp singularities, time-dependent evolution of small disturbances of the flat interface result in the formation of deep grooved cusps (also [Chiu and Gao]); experimental validation of sharp cusplike features in $SI_{0.6}$ $Ge_{0.4}$

zero contact-angle condition between the wetting layer and islands



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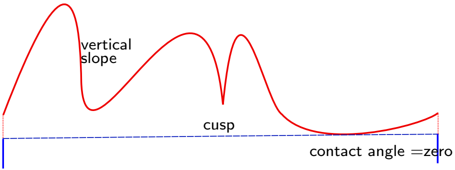

- conclude that the graph of h is a Lipschitz continuous curve away from a finite number of singular points (cusps, vertical cuts).
- ... and more: Lipschitz continuity of h +blow up argument+classical results on corner domains for solutions of **Lamé systems** of $h \Rightarrow$ decay estimate for the gradient of the displacement $\mathbf{u}$ near the boundary $\Rightarrow C^{1,\alpha}$ regularity of h and $\nabla \mathbf{u}$; bootstrap.

this takes us to linearly isotropic materials

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Linearly Isotropic Elastic Materials

$$W(\mathbf{E}) = \frac{1}{2}\lambda\,[\mathrm{tr}\,(\mathbf{E})]^2 + \mu\,\mathrm{tr}\left(\mathbf{E}^2\right)$$

λ and μ are the (constant) Lamé moduli

$$\mu > 0\,, \quad \mu + \lambda > 0\,.$$

Euler-Lagrange system of equations associated to W

$$\mu\Delta\mathbf{u} + (\lambda + \mu)\,\nabla\,(\mathrm{div}\,\mathbf{u}) = \mathbf{0} \quad \text{in } \Omega.$$

Regularity of Γ: No Corners

$$\Gamma_{\text{sing}} := \Gamma_{\text{cusps}} \cup \{(x, h(x)) : h(x) < h^-(x)\}$$

Already know that Γ_{sing} is finite.

Theorem

$(\mathbf{u}, \Omega) \in X \ldots \delta$-local minimizer for the functional F_∞.
Then $\Gamma \setminus \Gamma_{\text{sing}}$ is of class $C^{1,\sigma}$ for all $0 < \sigma < \frac{1}{2}$.

As an immediate corollary, get the zero contact-angle condition

Corollary

$(\mathbf{u}, \Omega) \in X \ldots$ local minimizer for the functional F_∞.
If $\mathbf{z}_0 = (x_0, 0) \in \Gamma \setminus \Gamma_{\text{sing}}$ then $h'(x_0) = 0$.

Shapes of Islands

With A. Pratelli and B. Zwicknagl

We proved that the shape of the island evolves with the size (and size varies with *misfit*! . . . later . . .):

small islands always have the half-pyramid shape, and as the volume increases the island evolves through a sequence of shapes that include more facets with increasing steepness – half pyramid, pyramid, half dome, dome, half barn, barn

This validates what was experimentally and numerically obtained in the physics and materials science literature

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Another incompatibility: miscut

Focus on small volume case. Small slope approximation ([Tersoff & Tromp, 1992; Spencer & Tersoff, 2010]):

$$E(u) \sim \int_0^W \int_0^W \log|x-y| u'(x) u'(y)\, dydx + \text{length}(\text{Graph}(u)) - W,$$

height profile u, $\text{supp}(h) = [0, W]$
fully facetted model:

$$u' \in \mathcal{A} := \{\tan(-\theta_m + n\theta) : \; n \in \mathcal{N} \subset \mathbb{Z}\}$$

- θ_m describes miscut. If $\theta_m \neq 0$, wetting not admissible

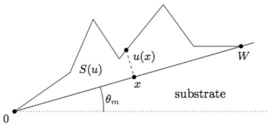

Figure: Sketch of a faceted height profile function u with support $[0, W]$. The profile is Lipschitz and the derivative lies almost everywhere in a discrete set. The miscut angle is denoted by $\theta_m \neq 0$, i.e., the preferred orientation of the film is not parallel to the substrate surface.

Compactness: bounds on the support of u

Set $\mathcal{F}(d) := \inf\{E(u) : \int u = d\}$

Theorem

- *For every* $d, r > 0$ *there exists* $\overline{W}$ *such that if* $E(u) \leq \mathcal{F}(d) + r$*, then* $W \leq \overline{W}$*.*
- *If* $d \to 0$ *and* $r \to 0$*, then* $\overline{W} \to 0$*.*
  $\to$ *no wetting effect for small volumes; wetting– optimal profiles tend to be extremely large and flat when the mass is small.*

Theorem

- *Every minimizer satisfies the quantized zero contact angle property*
- *There is a volume* $\overline{d} > 0$ *such that the half pyramid is the* *unique* *minimizer for every* $d \in (0, \overline{d})$*.*

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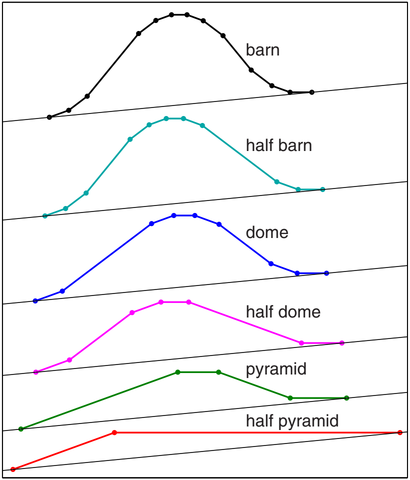

Figure: Shape transitions with increasing volume at miscut angle 3°. Numerical simulation. Courtesy of B. Spencer and J. Tersoff, *Appl. Phys. Lett.* bf 96/7, 073114 (2010)

Surface Diffusion in Epitaxially Strained Solids. The Context

With N. Fusco, G. Leoni, M. Morini

Einstein-Nernst volume preserving evolution law:

$$V = C\Delta_\Gamma \mu$$

V ... normal velocity of evolving interface x Δ_Γ ... tangential Laplacian

μ ... chemical potential, first variation of the free-energy functional

$$\int_{\Omega_h} W(\mathbf{E}(\mathbf{u}))\, \mathbf{dx} + \int_{\mathbf{\Gamma_h}} \varphi(\theta) \mathbf{d}\mathcal{H}^{\mathbf{1}}$$

$\varphi(\theta) = \psi(\cos\theta, \sin\theta)$ with $\psi(\xi) \sim |\xi| \in C^2$ away from the origin

ill-posed . . . so add a perturbation

Get (with $C = 1$)

$$V = ((\varphi_{\theta\theta} + \varphi)k + W(\mathbf{E}(\mathbf{u})))_{\sigma\sigma}$$

k . . . curvature of Γ_h
$(\cdot)_\sigma$ . . . tangential derivative
$u(\cdot, t)$ . . . elastic equilibrium in $\Omega_{h(\cdot,t)}$ under periodic b. c.

$$V = \left((\varphi_{\theta\theta} + \varphi)k + W(\mathbf{E}(\mathbf{u})) - \varepsilon\left(\mathbf{k}_{\sigma\sigma} + \frac{\mathbf{1}}{\mathbf{2}}\mathbf{k}^3\right)\right)_{\sigma\sigma}$$

H^{-1}- gradient flow for [Cahn and Taylor]; Wilmore

$$G(h) := \int_{\Omega_h} W(\mathbf{E}(\mathbf{u}))\,\mathbf{dx} + \int_{\Gamma_h}\left(\varphi(\theta) + \frac{\varepsilon}{\mathbf{2}}\mathbf{k}^2\right)\mathbf{d}\mathcal{H}^1$$

De Giorgi's minimizing movements: short time existence, uniqueness, regularity

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De Giorgi's minimizing movements: short time existence, uniqueness, regularity

u minimizes

$$v \mapsto F(v,h) := \int_{\Omega_h} W(\mathbf{E}(\mathbf{v}))\,\mathbf{dx} + \int_{\mathbf{\Gamma_h}} \left(\varphi(\theta) + \frac{\varepsilon}{\mathbf{2}}\mathbf{k^2}\right) \mathbf{d}\mathcal{H}^{\mathbf{1}}$$

among sufficiently regular v's such that

- $v(x,0) = (e_0 x, 0)$
- $v(\cdot,\cdot) - (e_0 x, 0)$ is b periodic

i.e.

$$v(x+b,y) - (e_0(x+b),0) = v(x,y) - (e_0,0)$$

for $x \in \mathbb{R}, 0 < y < h(x)$

Rätz, Ribalta, Voigt, without elasticity

What We Proved . . .

short time existence, uniqueness, and regularity of a spatially periodic solution of the Cauchy problem (for $b > 0$)

$$\begin{cases} \frac{1}{J}\frac{\partial h}{\partial t} = \Big((\varphi_{\theta\theta} + \varphi)k + W(\mathbf{E}(\mathbf{u})) - \varepsilon\big(\mathbf{k}_{\sigma\sigma} + \frac{1}{2}\mathbf{k}^3\big)\Big)_{\sigma\sigma}, \quad \text{in } \mathbb{R} \times [0, T_0], \\ \mathrm{Div}\mathbb{C}\mathbf{E} = \mathbf{0} \quad \text{in } \Omega_h, \\ \mathbb{C}\mathbf{E}(\mathbf{u})[\nu] = \mathbf{0} \quad \text{on } \Gamma_h, \qquad \mathbf{u}(\mathbf{x}, \mathbf{0}, \mathbf{t}) = \mathbf{e_0}(\mathbf{x}, \mathbf{0}), \\ h(\cdot, t) \text{ and } \nabla u(\cdot, t) \quad \text{are } b\text{-periodic} \\ h(\cdot, 0) = h_0 \end{cases}$$

e_0 . . . nonzero constant that reflects the mismatch between the crystalline lattices of the film and the substrate

$h : \mathbb{R} \times [0, T_0] \to (0, +\infty)$ . . . one-dimensional function describing the profile Γ_h of the film

$$J := \sqrt{1 + \left|\frac{\partial h}{\partial x}\right|^2} \quad \text{length factor of } \Gamma_h, \qquad k := -\frac{\partial}{\partial x}\left(\frac{\frac{\partial h}{\partial x}}{\sqrt{1 + \left|\frac{\partial h}{\partial x}\right|^2}}\right),$$

$W(\mathbf{E}(\mathbf{u})) = \frac{1}{2}\mathbb{C}\mathbf{E}(\mathbf{u}) : \mathbf{E}(\mathbf{u})$

$h_0 \in H^2_{loc}(\mathbb{R})$ . . . b-periodic function

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$W(\mathbf{E}(\mathbf{u})) = \frac{1}{2}\mathbb{C}\mathbf{E}(\mathbf{u}) : \mathbf{E}(\mathbf{u})$

$h_0 \in H^2_{loc}(\mathbb{R})$ ... b-periodic function

What We Proved ...

short time existence, uniqueness, and regularity of a spatially periodic solution of the Cauchy problem (for $b > 0$)

$$\begin{cases} \frac{1}{J}\frac{\partial h}{\partial t} = \Big((\varphi_{\theta\theta} + \varphi)k + W(\mathbf{E}(\mathbf{u})) - \varepsilon\big(\mathbf{k}_{\sigma\sigma} + \frac{1}{2}\mathbf{k}^3\big)\Big)_{\sigma\sigma}, \quad \text{in } \mathbb{R} \times [0, T_0], \\ \mathrm{Div}\mathbb{C}\mathbf{E} = \mathbf{0} \quad \text{in } \Omega_h, \\ \mathbb{C}\mathbf{E}(\mathbf{u})[\nu] = \mathbf{0} \quad \text{on } \Gamma_h, \qquad \mathbf{u}(\mathbf{x}, \mathbf{0}, \mathbf{t}) = \mathbf{e_0}(\mathbf{x}, \mathbf{0}), \\ h(\cdot, t) \text{ and } \nabla u(\cdot, t) \quad \text{are } b\text{-periodic} \\ h(\cdot, 0) = h_0 \end{cases}$$

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Strategy

Adopt De Giorgi's minimizing movements: construct discrete time evolutions by solving iteratively suitable minimum incremental problems. minimizing movements have been already successfully implemented to treat various mean curvature type flows without surface diffusion – e.g., Almgren, Taylor & Wang, Caselles & Chambolle, Bellettini, Caselles, Chambolle & Novaga

Start with a b-periodic initial datum $h_0 \in H^2_{loc}(\mathbb{R})$ and, given $T > 0$, $N \in \mathbb{N}$, for $i = 1, \ldots, N$, define inductively $h_{i,N}$ as the minimizer of

$$G(h) + \frac{1}{2\tau} d^2(h, h_{i-1,N})$$

$\tau := \frac{T}{N}$, d suitable H^{-1}-distance between h and $h_{i-1,N}$

what is the "right choice of d?

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The H^{-1} Distance

Given $T > 0$, $N \in \mathbb{N}$, set $\Delta T := \frac{T}{N}$. For $i = 1, \ldots, N$, define inductively $(h_{i,N}, u_{i,N})$ as the solution of the minimum problem

$$\min\left\{ F(h,u) + \frac{1}{2\Delta T} \int_{\Gamma_{h_{i-1,N}}} \left(\int_0^x \big(h(\zeta) - h_{i-1,N}(\zeta)\big)\, d\zeta \right)^2 d\mathcal{H}^1(x,y) : \right.$$

$$\left. \int_0^b h\, dx = \int_0^b h_0\, dx, \int_{\Gamma_{h_{i-1,N}}} \int_0^x (h(\zeta) - h_{i-1,N}(\zeta)) d\zeta\, d\mathcal{H}^1(x,y) = 0 \right\}$$

For $x \in \mathbb{R}$ and $(i-1)\Delta T \le t \le i\Delta T$, $i = 1, \ldots, N$, define

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

$u_N(\cdot,t)$ … elastic equilibrium corresponding to $h_N(\cdot,t)$
i.e. minimizer of the elastic energy in $\Omega_{h_N(\cdot,t)}$ among all admissible u

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Alternative Formulation of the Incremental Minimum Problem

$$\min\left\{ F(h,u) + \frac{1}{2\Delta T}\left\| \frac{h - h_{i-1,N}}{J_{i-1,N}} \right\|^2_{H^{-1}(\Gamma_{i-1,N})} : \ (h,u)\ \text{admissible} \right\}$$

$J_{i-1,N}$ denotes the length factor of $\Gamma_{i-1,N}$
$H^{-1}(\Gamma_{i-1,N})$-norm is defined as:

$$\|f\|^2_{H^{-1}(\Gamma)} = \left(\sup_{\|\varphi\|_{H^1(\Gamma)}=1} \int_\Gamma f\varphi \, d\mathcal{H}^1 \right)^2$$

$$= \int_\Gamma \left(F(z) - \fint_\Gamma F \, d\mathcal{H}^1 \right)^2 d\mathcal{H}^1(z) + \left(\int_\Gamma f \, d\mathcal{H}^1 \right)^2$$

where $F(z) := \int_{\Gamma(z_0,z)} f(w)\, d\mathcal{H}^1(w)$

Existence, Regularity, Uniqueness

Theorem

$h_0 \in H^2_\#(0, b)$ strictly positive. There exists T_0 s.t. evolution problem admits a weak solution in $[0, T_0]$ with initial datum h_0.

(i) $h \in C^{0,\beta}([0, T_0]; C^{1,\alpha}([0, b]))$ for all $\alpha \in (0, \frac{1}{2})$ and $\beta \in (0, \frac{1-2\alpha}{16})$;

(ii) $h \in L^2(0, T_0; H^4_\#(0, b))$;

(iii) if $\psi \in C^3(\mathbb{R}^2 \setminus \{0\})$ then $h \in L^2(0, T_0; H^5_\#(0, b))$;

(iv) if $\psi \in C^4$ away from the origin, $h_0 \in H^3_\#(0, b)$, $h_0 > 0$, then $h \in L^2(0, T_0; H^6_\#(0, b)) \cap H^1(0, T_0; L^2(0, b))$.

$\psi \in C^3(\mathbb{R}^2 \setminus \{0\})$, h_1, h_2 two weak solutions in $[0, T_0]$ with initial datum h_0. Then $h_1 = h_2$.

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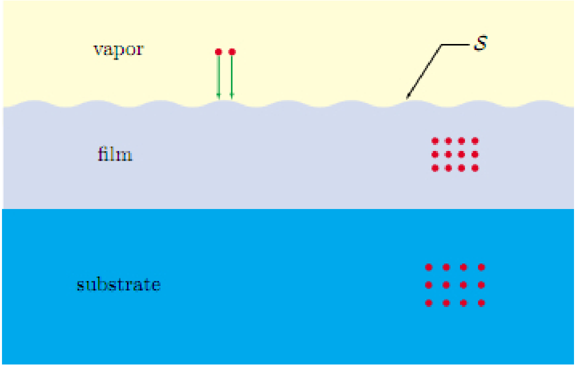
Proof

$$h_N \to h \quad \text{in} \quad L^{\frac{12}{5}}(0, T_0; C^{2,1}_{\#}([0,b])) \cap L^{\frac{24}{5}}(0, T_0; C^{1,1}_{\#}([0,b])) \ldots$$

P. Piovano: Evaporation-Condensation

The profile of the film is modeled as a grain-vapor interface with the vapor being considered as a reservoir that interacts with the profile of the film only through the evaporation-condensation process



Mullins: Evaporation-Condensation

derived the equations that describe the planar motion of isotropic grain boundaries by evaporation-condensation: Up to a rescaling (motion by mean curvature - elastic bulk energy)

$$V = (\varphi_{\theta\theta} + \varphi)k - W(\mathbf{E}(\mathbf{u}))$$

Piovano undertook a similar analysis via De Giorgi's minimizing movements

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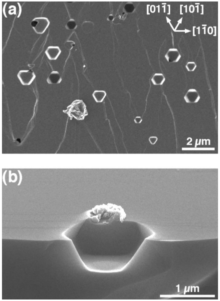
Material Voids . . . Pits? The Context

With N. Fusco, G. Leoni and V. Millot

material voids: Colin, Siegel, Miksis, Voorhees, Suo, Wang



Voids in UO_2. Courtesy of M. Castell (2003)

The Model

$$F(u,V) := \int_{B_0 \setminus V} \mathbb{C}(\mathbf{E}(u)) \cdot \mathbf{E}(u)\, dx + \int_{\partial V} \varphi(\nu^i)\, ds,$$

- $u : B_0 \setminus V \to \mathbb{R}^2$ ... planar displacement
- $\mathbf{E}(u)$ ... symmetrized strain (2 D Linear Elasticity)

$$\mathbf{E}(u) := \frac{1}{2}\left(\nabla u + (\nabla u)^T\right),$$

- $\mathbb{C}$ positive definite fourth-order tensor,

$$\mathbb{C}(\mathbf{E}) \cdot \mathbf{E} > 0 \text{ for all symmetric matrices } \mathbf{E} \neq \mathbf{0},$$

- $B_0 \subset \mathbb{R}^2$ fixed large ball, $V \subset B_0$ material void

  V closed, star-shaped, $|V| = d > 0$ fixed, ∂V Lipschitz,

- $\varphi : \mathbb{R}^2 \to [0,\infty)$ positively 1-homogeneous, Lipschitz, ν^i inner normal to ∂V.

$$F(u, V) := \int_{B_0 \setminus V} \mathbb{C}(\mathbf{E}(u)) \cdot \mathbf{E}(u)\, dz + \int_{\partial V} \varphi(\nu^i)\, ds.$$

Define X_{Lip} to be the family of all pairs (u, V) such that

- $V \ldots$ closed, star-shaped, $|V| = d > 0$ fixed, ∂V Lipschitz
- $u \in H^1_{\text{loc}}\left(\mathbb{R}^2 \setminus V; \mathbb{R}^2\right)$, $u = u_0$ a.e. in $\mathbb{R}^2 \setminus B_0$.

Problem

Minimize F over all $(u, V) \in X_{\text{Lip}}$.

Here $u_0 : \mathbb{R}^2 \to \mathbb{R}^2$ fixed, Lipschitz, determines the mismatch and forces stress

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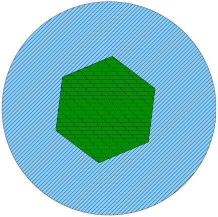
$$F(u,V) := \int_{B_0 \setminus V} \mathbb{C}(\mathbf{E}(u)) \cdot \mathbf{E}(u)\, dz + \int_{\partial V} \varphi(\nu^i)\, ds.$$

The formulation follows Siegel, Miksis and Voorhees (2004) with:

- $B_0 \setminus V$ in place of $\mathbb{R}^2 \setminus V$
- $u = u_0$ a.e. in $B_0 \setminus V$ in place of

$$\mathbb{C}(\mathbf{E}(u)) \to \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} \qquad \text{as } \sqrt{x^2 + y^2} \to \infty$$



void in an elastic solid

Goals

$$F(u,V) := \int_{B_0 \setminus V} \mathbb{C}(\mathbf{E}(u)) \cdot \mathbf{E}(u)\, dz + \int_{\partial V} \varphi(\nu^i)\, ds.$$

Consider

$$\min_{(u,V)\in X_{\text{Lip}}} F(u,V) \qquad \text{(P)}$$

- Existence of minimizers of (P)
- Regularity of minimizers of (P).

Existence of Minimizers

Consider minimizing sequence $(u_n, V_n) \in X_{\text{Lip}}$ such that

$$\lim_{n\to\infty} F(u_n, V_n) = \inf_{(u,V)\in X_{\text{Lip}}} F(u, V).$$

Then

$$\sup_n \int_{B_0 \setminus V_n} |\mathbf{E}(u_n)|^2 \, dz < \infty, \quad \sup_n \text{length}\, \partial V_n < \infty.$$

Up to a subsequence

- $V_n \to V$ in the Hausdorff metric

Braides, Chambolle and Solci, L^1 convergence

- $u_n \rightharpoonup u$ in $H^1(\omega; \mathbb{R}^2)$ for all $\omega \Subset \mathbb{R}^2 \setminus V$

for some

- $V \subset B_0$ closed, star-shaped, $|V| = d > 0$, V finite perimeter,
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X … space of all such (u, V) with these properties

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X . . . space of all such (u, V) with these properties

Relaxation

But F is not lower semicontinuous. Consider the relaxed energy

$$\mathcal{F}(u,V) := \inf\left\{\liminf_{n\to\infty} F(u_n,V_n) : (u_n,V_n) \in X_{\text{Lip}}, (u_n,V_n) \to (u,V)\right\}$$

Assume φ convex and V star-shaped w.r.t. 0.

Theorem (Fusco, Fonseca, G.L., & Millot)

$$\mathcal{F}(u,V) = \int_{B_0\setminus V} \mathbb{C}(\mathbf{E}(u))\cdot\mathbf{E}(u)\,dz + \int_{\partial^* V} \varphi\left(\nu^i\right)\,ds$$
$$+ \int_{\text{cuts}} \left(\varphi\left(\nu^i\right) + \varphi\left(-\nu^i\right)\right)\,ds \quad \textit{for } (u,V)\in X$$

Regularity of Minimizers

$$\mathcal{F}(u,V) = \int_{B_0\setminus V} \mathbb{C}(\mathbf{E}(u))\cdot\mathbf{E}(u)\,dz + \int_{\partial^* V} \varphi\left(\nu^i\right)\,ds$$
$$+ \int_{\text{cuts}} \left(\varphi\left(\nu^i\right) + \varphi\left(-\nu^i\right)\right)\,ds.$$

Since $\mathcal{F}$ is lower semicontinuous, there exists $(u,V)\in X$ such that

$$\mathcal{F}(u,V) = \min_{(u',V')\in X} \mathcal{F}\left(u',V'\right) = \inf_{(u',V')\in X_{\text{Lip}}} F\left(u',V'\right). \qquad \text{(R)}$$

Regularity of (u,V) ?

- Wulff set of φ is a polygon
- Wulff set of φ is smooth

Regularity of Minimizers

$$\mathcal{F}(u,V) = \int_{B_0 \setminus V} \mathbb{C}(\mathbf{E}(u)) \cdot \mathbf{E}(u)\, dz + \int_{\partial^* V} \varphi\left(\nu^i\right)\, ds + \int_{\text{cuts}} \left(\varphi\left(\nu^i\right) + \varphi\left(-\nu^i\right)\right)\, ds.$$

Since $\mathcal{F}$ is lower semicontinuous, there exists $(u,V) \in X$ such that

$$\mathcal{F}\left(u,V\right) = \min_{(u',V') \in X} \mathcal{F}\left(u',V'\right) = \inf_{(u',V') \in X_{\text{Lip}}} F\left(u',V'\right). \qquad \text{(R)}$$

Regularity of (u,V) ?

- Wulff set of φ is a polygon
- Wulff set of φ is smooth

The Exterior Wulff Condition

Wulff set of φ,

$$W := \left\{ w \in \mathbb{R}^2 : \varphi^\circ(w) < 1 \right\}$$

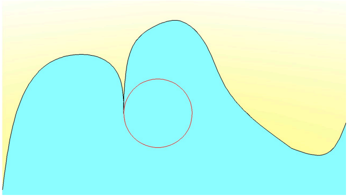
where φ° polar function of φ, i.e.,

$$\varphi^\circ(w) := \max_{|z|=1} \frac{z \cdot w}{\varphi(z)}, \quad w \in \mathbb{R}^2.$$

Theorem (Fusco, Fonseca, G.L., & Millot)

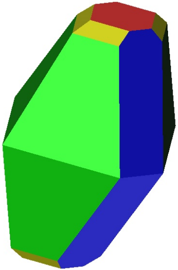
Let $(u, V) \in X$ be a minimizer of (R). Then there is $\varrho_0 > 0$ such that for all $z \in \partial V$ there is $w \in \mathbb{R}^2$ such that $w + \varrho_0 W \subset \mathbb{R}^2 \setminus V$ and $z \in \partial (w + \varrho_0 W)$.

Interior Sphere Condition:



Chambolle and Larsen (2003), when the Wulff shape is the ball
Fonseca, Fusco, G. L., and Morini (2007)

The Polygonal Case



Sulfur http://www.ctcms.nist.gov

The Polygonal Case

Theorem (Fusco, Fonseca, G.L., & Millot)

Assume that the Wulff set W is a polygon with internal angles greater than $\frac{\pi}{2}$. Let $(u, V) \in X$ be a minimizer of (R). Then ∂V is the union of finitely many Lipschitz graphs.

$$V^+ := \left\{(r\cos\theta, r\sin\theta) : \theta \in [0, 2\pi]\,,\ 0 \leq r \leq \rho_V^+(\theta)\right\}.$$

- $V = V^+ \cup$ cuts, only finitely many cuts
- there is a finite set $\Gamma_{\text{sing}} \subset \partial V^+$ such that if $z \in \partial V^+ \setminus \Gamma_{\text{sing}}$, then near z the set ∂V is the graph of a Lipschitz function
- if $z \in \Gamma_{\text{sing}}$, $z \neq 0$, then near z, the set $\partial V \backslash$cuts is the union of two graphs of Lipschitz functions intersecting only at z
- if $0 \in \Gamma_{\text{sing}}$, then near 0, the set ∂V is the union of at most six graphs of Lipschitz functions intersecting only at 0

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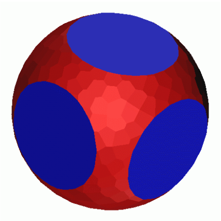
The Smooth Case



Isotropic: http://www.ctcms.nist.gov

Theorem (Fusco, Fonseca, G.L., & Millot)

Assume that the Wulff set W is of class C^1. Let $(u, V) \in X$ be a minimizer of (R). Then except for a finite number of points $\partial V \setminus \mathrm{cuts}$ is of class C^1.

$$V^+ := \left\{(r\cos\theta, r\sin\theta) : \theta \in [0, 2\pi], \ 0 \le r \le \rho_V^+(\theta)\right\}.$$

- $V = V^+ \cup \mathrm{cuts}$, only finitely many cuts
- there is a finite set $\Gamma_{\mathrm{cusp}} \subset \partial V^+$ such that if $z \in \partial V^+ \setminus \Gamma_{\mathrm{cusp}}$, then near z the set ∂V is the graph of a C^1 function
- if $z \in \Gamma_{\mathrm{cusp}}$, then near z, the set $\partial V \setminus \mathrm{cuts}$ is the union of two graphs of Lipschitz functions intersecting only at z and differentiable at z

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- $V = V^+ \cup \text{cuts}$, only finitely many cuts
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Bonacini and Piovano

Recently they proved regularity results in the context of material voids in elastic solids that hold true for any dimension and without the restriction that the voids are starshaped