Quantum Dots and Dislocations: Dynamics of Materials Defects

most in collaboration with N. Fusco, G. Leoni and M. Morini

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Supported by the National Science Foundation (NSF)

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Outline

- Quantum Dots: Wetting and zero contact angle. Shapes of islands
- Surface Diffusion in epitaxially strained solids: Existence and regularity
- Nucleation of Dislocations: Release of energy . . . and film becomes flat!

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Quantum Dots. The Context

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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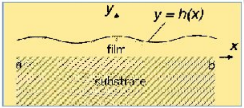
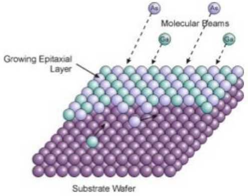
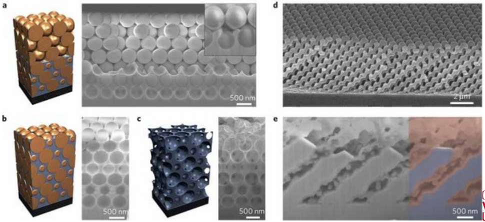
Islands

To release some of the elastic energy due to the strain: atoms on the free surface rearrange and morphologies such as formation of islands (*quatum dots*) of pyramidal shapes are energetically more economical. Kinetics of Stranski-Krastanow depend on initial thickness of film, competition between strain and surface energies, anisotropy, ETC.







3D photonic crystal template partially filled with GaAs by epitaxy.

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Why Do We Care?

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.

• **3D Printing:** New additive manufacturing technology– the mathematical understanding of the theory of dislocations will be central to address the energy balance between laser beam power (laser beams are used to melt the powder of the material into a specific shape) and the energy required to form a given geometrical shape

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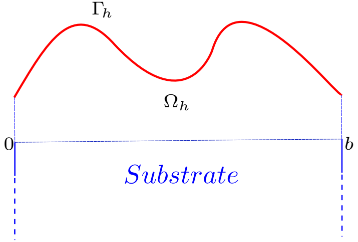
Epitaxial films: equilibrium configurations



- $E(u) = \frac{1}{2}(\nabla u + \nabla^T u)$ ... strain
- $W(E) = \frac{1}{2} E \cdot \mathbb{C} E$ ... energy density
- $\mathbb{C}$ ... positive definite fourth-order tensor
- $\psi =$ ... (anisotropic) surface energy density
- $u(x,0) = e_0(x,0), \ \ \nabla u(\cdot, t)$ ... Q-periodic

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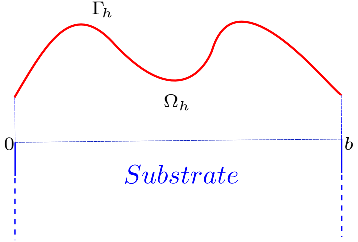

$$F(h,u) := \int_{\Omega_h} W(E(u))\,dxdy + \int_{\Gamma_h} \psi(\nu)d\sigma$$

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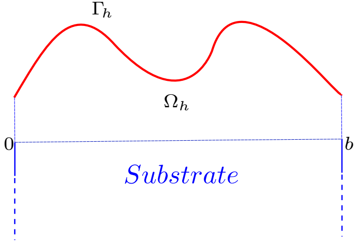

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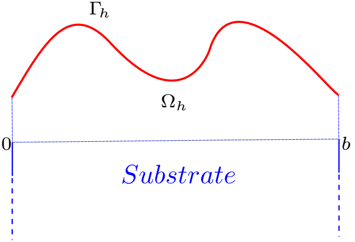

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$$\inf \{F(h,u) : \ (h,u) \text{ admissible}, \ |\Omega_h| = d\}$$

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$$F(h,u) := \int_{\Omega_h} W(E(u))\,dxdy + \int_{\Gamma_h} \psi(\nu)d\sigma$$

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)

$$E_0\left(y\right) = \begin{cases} e_0 \mathbf{i}\otimes\mathbf{i} & \text{if } y \geq 0, \\ 0 & \text{if } y < 0, \end{cases}$$

$e_0 > 0$

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

elastic energy per unit area: $W\left(E - E_0\left(y\right)\right)$

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

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

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

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

Total energy of the system:

$$F(u, \Omega_h) := \int_{\Omega_h} W\left(E(u)(x,y) - E_0(y)\right) d\mathbf{x} + \int_{\Gamma_h} \psi(y)\, d\mathcal{H}^1(\mathbf{x}),$$

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

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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")

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

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

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

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smooth transition – total energy of the system:

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

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

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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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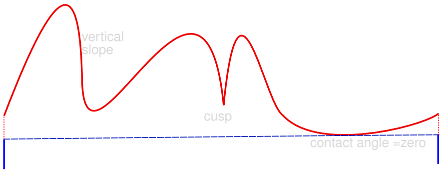
Cusps and Vertical Cuts

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 $\mathrm{SI}_{0.6}$ $\mathrm{Ge}_{0.4}$

zero contact-angle condition between the wetting layer and islands



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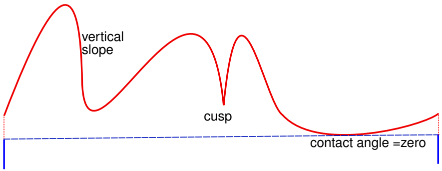

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Regularity . . .

- 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 leads us to linearly isotropic materials

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Linearly Isotropic Elastic Materials

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

λ and μ are the (constant) Lamé moduli

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

Euler-Lagrange system of equations associated to W

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

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Regularity of Γ: No Corners

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

Already know that $\Gamma_{\rm sing}$ is finite

Theorem

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

If $\mathbf{z}_0 = (x_0, 0) \in \Gamma \setminus \Gamma_{\rm sing}$ then $h'(x_0) = 0$.

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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

Small slope approximation of a geometrically linear elastic strain energy ([Tersoff & Tromp, 1992; Spencer & Tersoff, 2010])

fully facetted model:

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

height profile u, supp$(u) = [0, L]$

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

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

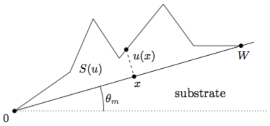

Figure : Sketch of a faceted height profile function u with support $[0, L]$. The profile is Lipschitz and the derivative lies almost everywhere in a discrete set. The miscut angle is denoted by $\theta_m \neq 0$, i.e., the preferred orientation of the film is not parallel to the substrate surface.

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Compactness: Bounds on the Support of u

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

Theorem

- *For every $d, r > 0$ there exists $\overline{L}$ such that if $E(u) \leq \mathcal{F}(d) + r$, then $L \leq \overline{L}$*
- *If $d \to 0$ and $r \to 0$, then $\overline{L} \to 0$*
  no wetting effect for small volumes; wetting– optimal profiles tend to be extremely large and flat when the mass is small. The flat profile is not admissible

Theorem

- *Every minimizer satisfies the quantized zero contact angle property: the island meets the substrate at the smallest angle possible*
- *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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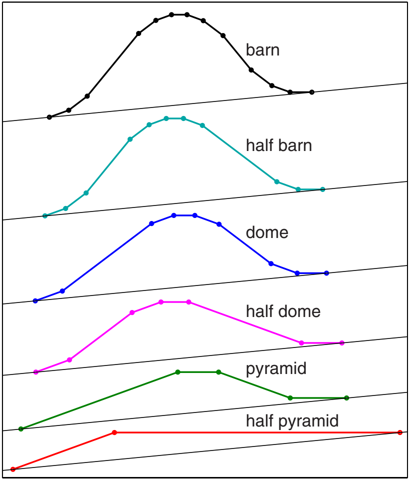

Figure : Shape transitions with increasing volume at miscut angle 3°. Numerical simulation. Courtesy of B. Spencer and J. Tersoff, *Appl. Phys. Lett.* bf 96/7, 073114 (2010)

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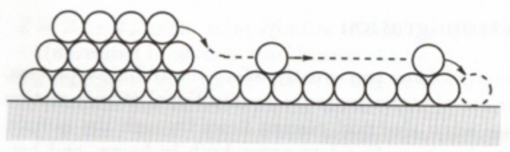
Surface Diffusion in Epitaxially Strained Solids [With N. Fusco, G. Leoni, M. Morini]



Einstein-Nernst Law : surface flux of atoms $\propto \nabla_\Gamma \mu$

μ= chemical potential $\rightsquigarrow$

$V = c \times \underbrace{\Delta_{\Gamma(t)}\mu}_{\text{Laplace-Beltrami operator}}$ (volume preserving)

μ= first variation of energy = $\underbrace{\mathrm{div}_\Gamma D\psi(\nu)}_{\text{anisotropic curvature}} + W(E(u)) + \lambda$

$$V = \Delta_\Gamma\Big(\mathrm{div}_\Gamma D\psi(\nu) + W(E(u))\Big)$$

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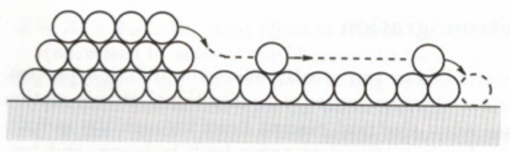

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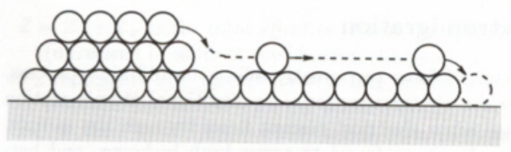

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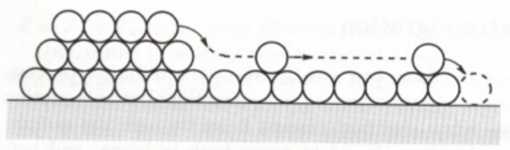

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$V = c \times \underbrace{\Delta_{\Gamma(t)}\mu}$ (volume preserving)

Laplace-Beltrami operator

μ= first variation of energy = $\underbrace{\mathrm{div}_\Gamma D\psi(\nu)}$ $+W(E(u)) + \lambda$

anisotropic curvature

$$V = \Delta_\Gamma \Big(\mathrm{div}_\Gamma D\psi(\nu) + W(E(u)) \Big)$$

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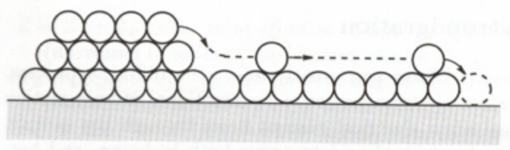

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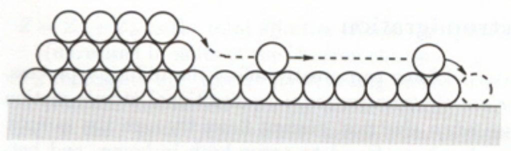
Surface Diffusion in Epitaxially Strained Solids [With N. Fusco, G. Leoni, M. Morini]



Einstein-Nernst Law : surface flux of atoms $\propto \nabla_\Gamma \mu$

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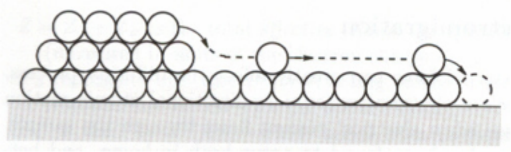

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Highly Anisotropic Surface Energies

For highly anisotropic ψ it may happen

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

$$\Downarrow$$

the evolution becomes backward parabolic

Idea: add a curvature regularization

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$$F(h,u) := \int_{\Omega_h} W(E(u))\,dxdy + \int_{\Gamma_h} \Big(\psi(\nu) + \frac{\varepsilon}{p}|H|^p\Big)d\sigma, \quad p > 2,\ \varepsilon > 0$$

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Highly Anisotropic Surface Energies in 2D

Regularized energy:

$$F(h,u) := \int_{\Omega_h} W(E(u))\,dxdy + \int_{\Gamma_h} \left(\psi(\nu) + \frac{\varepsilon}{2}k^2\right) d\mathcal{H}^1$$

Why here $p > 2$: technical . . . in two dimensions, the Sobolev space $W^{2,p}$ embeds into $C^{1,(p-2)/p}$ if $p > 2$

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- F., Fusco, Leoni, and Morini (ARMA 2012): evolution of films in two-dimensions
- F., Fusco, Leoni, and Morini (To appear in Analysis & PDE): evolution of films in three-dimensions

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- In the context of grain growth, curvature regularization was proposed by Di Carlo, Gurtin, Podio-Guidugli (1992)
- In the context of epitaxial growth, see Gurtin & Jabbour (2002)

Given Q, find $h\colon \mathbb{R}^2 \times [0,T_0] \to (0,+\infty)$ s.t.

$$\begin{cases} \dfrac{1}{J}\dfrac{\partial h}{\partial t} = \Delta_\Gamma \Big[\mathrm{div}_\Gamma (D\psi(\nu)) + W(E(u)) \\ \qquad\qquad -\varepsilon \Big(\Delta_\Gamma (|H|^{p-2}H) - |H|^{p-2}H \Big(\kappa_1^2 + \kappa_2^2 - \dfrac{1}{p}H^2\Big)\Big)\Big], \quad \text{in } \mathbb{R}^2 \times (0,T_0) \\ \mathrm{div}\, \mathbb{C}E(u) = 0 \quad \text{in } \Omega_h \\ \mathbb{C}E(u)[\nu] = 0 \quad \text{on } \Gamma_h, \qquad u(x,0,t) = e_0(x,0) \\ h(\cdot,t) \text{ and } Du(\cdot,t) \quad \text{are } Q\text{-periodic} \\ h(\cdot,0) = h_0 \end{cases}$$

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- Rätz, Ribalta, Voigt (2006): numerical results for the diffuse interface version of the evolution
- Garcke: analytical results concerning some diffuse interface versions of the evolution equation
- Bellettini, Mantegazza, Novaga (2007): analytical results concerning the L^2-gradient flow of higher order geometric functionals (without elasticity)
- Elliott & Garcke (1997), Escher, Mayer & Simonett (1998): existence results for the surface diffusion equation without elasticity and without curvature regularization, via semigroups techniques
- no analytical results for the sharp interface evolution with elasticity

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The Gradient Flow Structure

- The evolution law is the gradient flow of the reduced energy $\overline{F}$ w.r.t a suitable H^{-1}-Riemannian structure

- Consider the "manifold"

$$\mathcal{M} := \left\{ \Omega_h : h \text{ is } Q-\text{periodic}, \int_Q h = d \right\}$$

- The tangent space of admissible normal velocities is

$$\mathcal{T}_{\Omega_h} M := \left\{ V : \Gamma_h \to \mathbb{R} : V \; Q\text{-periodic}, \int_{\Gamma_h} V = 0 \right\},$$

endowed with the H^{-1}-scalar product

$$g_{\Omega_h}(V_1, V_2) := \int_{\Gamma_h} \nabla_{\Gamma_h} w_1 \nabla_{\Gamma_h} w_2 \, d\sigma \qquad \text{for all } V_1, V_2 \in T_{\Omega_h}\mathcal{M},$$

where w_i, $i = 1, 2$, is the solution to

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Minimizing Movements Approach to Gradient Flows

- H Hilbert space
- $F : H \to \mathbb{R}$, F of class C^1

$$\begin{cases} \dot{u} = -\nabla_H F(u) \\ u(0) = u_0 \end{cases}$$

Semi-implicit time-discretization: Set $w_0 := u_0$ and let w_i the solution to

$$\min_{w \in H} \left\{ F(w) + \frac{1}{2\tau} \|w - w_{i-1}\|_H^2 \right\}$$

The discrete evolution converges to the continuous evolution as $\tau \to 0$

- This approach can be generalized to metric spaces $\rightsquigarrow$ De Giorgi's minimizing movements
- In the context of geometric flows $\rightsquigarrow$ Almgren-Taylor-Wang.

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The Minimizing Movements Scheme in Our Case

- Given $T > 0$, $N \in \mathbb{N}$, we set $\tau := \frac{T}{N}$. For $i = 1, \ldots, N$ we define inductively (h_i, u_i) as the solution of the incremental minimum problem

$$\min_{\substack{(h,u)\ \text{admissible} \\ \|Dh\|_\infty \leq C}} F(h,u) + \frac{1}{2\tau}\int_{\Gamma_{h_{i-1}}} |D_{\Gamma_{h_{i-1}}} w_h|^2 d\mathcal{H}^2$$

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The Discrete Euler-Lagrange Equation

- The Euler-Lagrange equation of the incremental problem is

$$\frac{1}{\tau} w_{h_i} = \mathrm{div}_{\Gamma_{h_i}}(D\psi(\nu)) + W(E(u_i)) - \varepsilon\Big(\Delta_{\Gamma_{h_i}}(|H_i|^{p-2}H_i) - |H_i|^{p-2}H_i\Big((\kappa_1^i)^2 + (\kappa_2^i)^2 - \frac{1}{p}H_i^2\Big)\Big)$$

- By applying $\Delta_{\Gamma_{h_{i-1}}}$ to both sides, we formally get

$$\frac{1}{J_{i-1}} \frac{h_i - h_{i-1}}{\tau} = \Delta_{\Gamma_{h_{i-1}}}\Big[\mathrm{div}_{\Gamma_{h_i}}(D\psi(\nu)) + W(E(u_i)) - \varepsilon\Big(\Delta_{\Gamma_{h_i}}(|H_i|^{p-2}H_i) - |H_i|^{p-2}H_i\Big((\kappa_1^i)^2 + (\kappa_2^i)^2 - \frac{1}{p}H_i^2\Big)\Big)\Big]$$

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Estimates

- $h_N(\cdot,t) = h_{i-1} + \frac{t-(i-1)\tau}{\tau}(h_i - h_{i-1})$ if $(i-1)\tau \le t \le i\tau$

Basic energy estimate:

$$F(h_i,u_i) + \frac{1}{2\tau}\int_{\Gamma_{h_{i-1}}} |D_{\Gamma_{h_{i-1}}} w_h|^2 d\mathcal{H}^2 \le F(h_{i-1},u_{i-1})$$

$$\rightsquigarrow \sum_{i=1}^N \frac{1}{2\tau}\|h_i - h_{i-1}\|^2_{H^{-1}} \le \sum_{i=1}^N \big(F(h_{i-1},u_{i-1}) - F(h_i,u_i)\big) \le CF(h_0,u_0)$$

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$\{h_N\}$ is bounded in $H^1(0,T;H^{-1})$

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Local in Time Existence of Weak Solutions

- Previous estimates+interpolation inequalities+higher regularity+ compactnes argument $\rightsquigarrow h_N \to h$ (up to a subsequence)
- h is a weak solution in the following sense:

Theorem (Local existence)

$h \in L^\infty(0,T_0;W^{2,p}_\#(Q)) \cap H^1(0,T_0;H^{-1}_\#(Q))$ is a weak solution in $[0,T_0]$ in the following sense:

(i) $\mathrm{div}_\Gamma(D\psi(\nu)) + W(E(u)) - \varepsilon\Big(\Delta_\Gamma(|H|^{p-2}H) - \frac{1}{p}|H|^p H + |H|^{p-2}H|B|^2\Big) \in L^2(0,T_0;H^1_\#(Q))$,

(ii) *for a.e.* $t \in (0,T_0)$

$$\frac{1}{J}\frac{\partial h}{\partial t} = \Delta_\Gamma\Big[\mathrm{div}_\Gamma(D\psi(\nu)) + W(E(u)) - \varepsilon\Big(\Delta_\Gamma(|H|^{p-2}H) - |H|^{p-2}H\Big(\kappa_1^2 + \kappa_2^2 - \frac{1}{p}H^2\Big)\Big)\Big] \quad \text{in } H^{-1}_\#(Q).$$

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Uniqueness and regularity in 2D

Theorem

In two dimensions:

(i) *The weak solution is unique.*

(ii) *If $h_0 \in H^3$, $\psi \in C^4$, then the solution is in $H^1(0,T_0;L^2) \cap L^2(0,T_0;H^6)$.*

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Global in Time Existence and Asymptotic Stability

Consider the regularized surface diffusion equation

$$\frac{1}{J}\frac{\partial h}{\partial t} = \Delta_\Gamma \Big[\operatorname{div}_\Gamma (D\psi(\nu)) + W(E(u)) - \varepsilon\Big(\Delta_\Gamma(|H|^{p-2}H) - |H|^{p-2}H\Big(\kappa_1^2 + \kappa_2^2 - \frac{1}{p}H^2\Big)\Big)\Big]$$

Detailed analysis of *Asaro-Tiller-Grinfeld morphological stability/instability* by Bonacini, and F., Fusco, Leoni and Morini:
• if d is sufficiently small, then the flat configuration (d, u_d) is a volume constrained local minimizer for the functional

$$G(h,u) := \int_{\Omega_h} W(E(u))\,dz + \int_{\Gamma_h} \psi(\nu)\,d\mathcal{H}^2\,.$$

d small enough $\Rightarrow$ the second variation $\partial^2 G(d, u_d)$ is positive definite $\Rightarrow$ local minimality property.

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Global in Time Existence and Asymptotic Stability – Main Result

Theorem

Assume that $D^2\psi(e_3) > 0$ *on* $(e_3)^\perp$ *and* $\partial^2 G(d, u_0) > 0$. *There exists* $\varepsilon > 0$ *s.t. if* $\|h_0 - d\|_{W^{2,p}} \leq \varepsilon$ *and* $\int_Q h_0 = d$, *then:*

(i) *any variational solution* h *exists for all times;*

(ii) $h(\cdot, t) \to d$ *in* $W^{2,p}$ *as* $t \to +\infty$.

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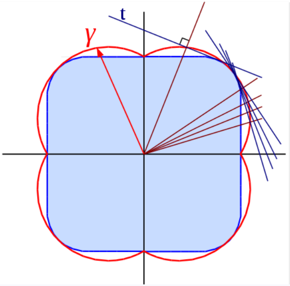
Liapunov Stability in the Highly Non-Convex Case

Consider the Wulff shape

$$W_\psi := \{z \in \mathbb{R}^3 : \ z \cdot \nu < \psi(\nu) \text{ for all } \nu \in S^2\}$$



Theorem (F.-Fusco-Leoni-Morini)

Assume that W_ψ contains a horizontal facet. Then for every $d > 0$ the flat configuration (d, u_d) is Liapunov stable, that is, for every $\sigma > 0$ there exists $\delta(\sigma) > 0$ s.t.

$$\int_Q h_0 = d, \quad \|h_0 - d\|_{W^{2,p}} \leq \delta(\sigma) \quad \Longrightarrow \quad \|h(t) - d\|_{W^{2,p}} \leq \sigma \text{ for all } t > 0.$$

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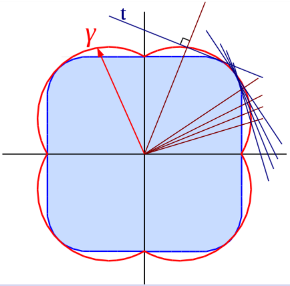

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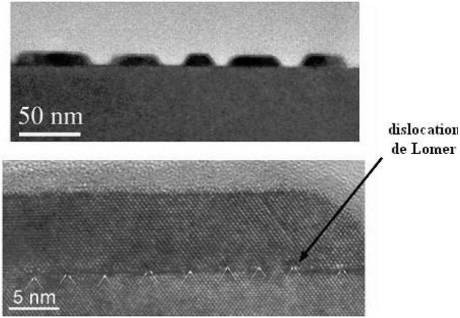
And Now . . . Epitaxy and Dislocations

lattice-mismatched semiconductors — formation of a periodic dislocation network at the substrate/layer interface



nucleation of dislocations is a mode of strain relief for sufficiently thick films

• when a cusp-like morphology is approached as the result of an increasingly greater stress in surface valleys, it is energetically favorable to nucleate a dislocation in the surface valley

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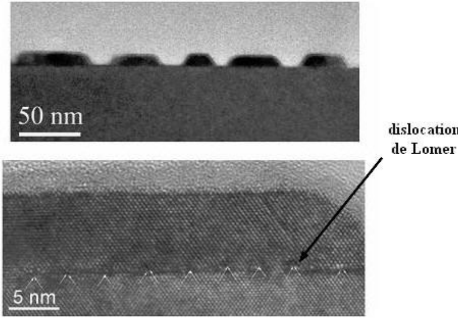

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Microscopic Level

- Perfect crystals

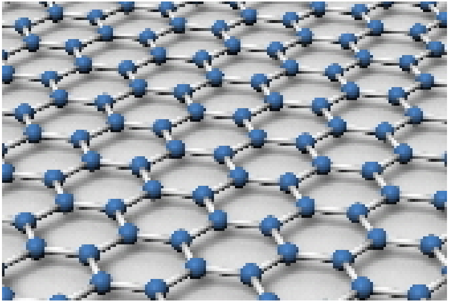

Figure : Courtesy of James Hedberg

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Microscopic Level

- Defects in crystalline materials

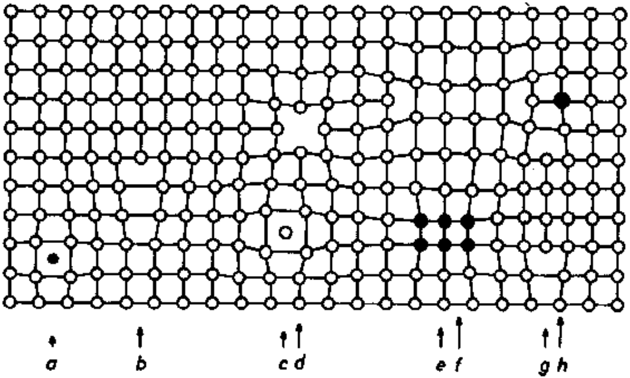

Figure : Courtesy of Helmut Föll

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Microscopic Level

- Line defects in crystalline materials. Orowon (1934); Polanyi (1934), Taylor (1934).

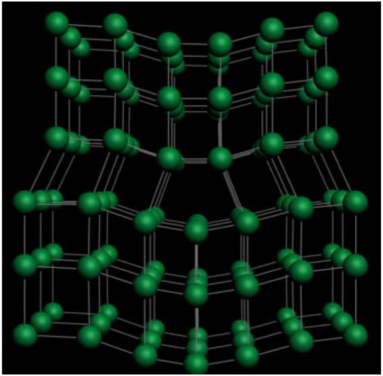

Figure : Courtesy of NTD

Microscopic Level

- Edge dislocations,
- Burgers vector, Burgers (1939)
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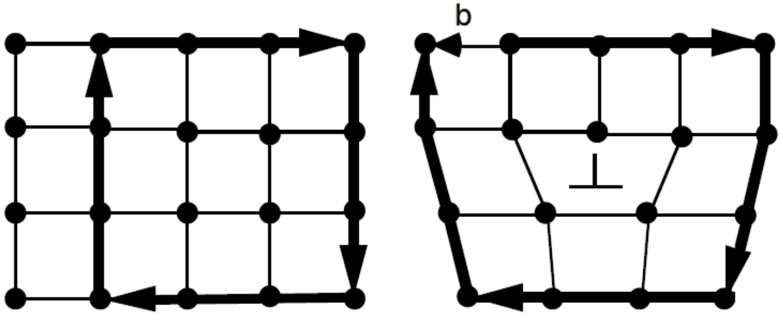

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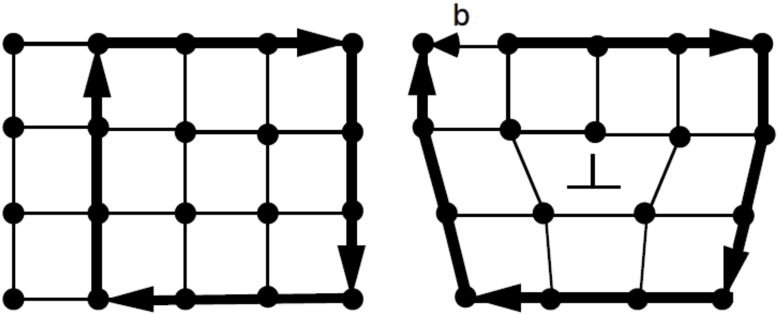

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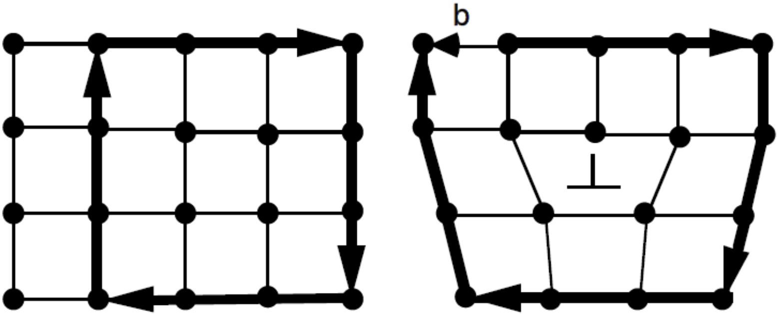

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Microscopic Level

- Screw dislocations
- Burgers vector

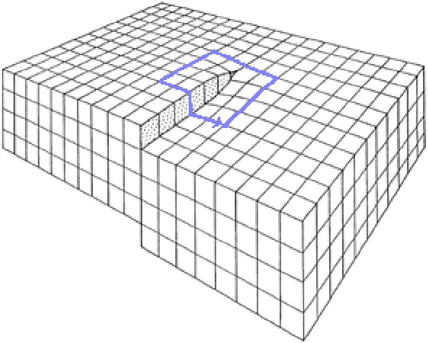

Figure : Courtesy of Helmut Föll

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Microscopic Level

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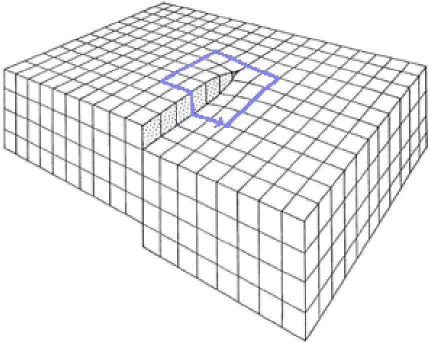

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Epitaxy and Dislocations: The Model

The Energy: vertical parts and cuts may appear in the (extended) graph of h

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

$\Sigma_h := \{(x,y) :\ x \in [0,b),\ h(x) < y < \min\{h(x-), h(x+)\}\}$ set of vertical cuts

$h(x\pm)$ ...the right and left limit at x

...now with the presence of isolated misfit dislocations in the film

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Epitaxy and Dislocations: The Model With Dislocations

System of Dislocations located at $z_1, \dots, z_k$ with Burgers Vectors $\mathbf{b}_1, \dots, \mathbf{b}_k$

$$\operatorname{curl} H = \sum_{i=1}^{k} \mathbf{b}_i \delta_{z_i}$$ strain field compatible with the system of dislocations

the elastic energy associated with such a singular strain is infinite!

Strategy:

- remove a core $B_{r_0}(z_i)$ of radius $r_0 > 0$ around each dislocation

OR

- regularize the **dislocation measure** $\sigma := \sum_{i=1}^{k} \mathbf{b}_i \delta_{z_i}$ through a convolution procedure

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Epitaxy and Dislocations: More on the Model With Dislocations

$$\operatorname{curl} H = \sigma * \rho_{r_0}\,. \quad \rho_{r_0} := (1/r_0^2)\rho(\cdot/r_0)$$ standard mollifier

Total energy associated with a profile h, a dislocation measure σ and a strain field H

$$F(h,\sigma,H) := \int_{\Omega_h} \left[\mu|H_{sym}|^2 + \frac{\lambda}{2}(\mathrm{tr}(H))^2\right] dz + \gamma\mathcal{H}^1(\Gamma_h) + 2\gamma\mathcal{H}^1(\Sigma_h)\,.$$

What we ask : Assume that a finite number k of dislocations, with given Burgers vectors $\mathbf{B} := \{\mathbf{b}_1,\dots,\mathbf{b}_k\} \subset \mathbb{R}^2$, are already present in the film

Optimal Configuration?

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What We Know

Theorem

The minimization problem

$$\min\{F(h,\sigma,H) : (h,\sigma,H) \in X(e_0;\mathbf{B}), \, |\Omega_h| = d\} \, .$$

admits a solution.

The equilibrium profile h satisfies the same regularity properties as in the dislocation-free case:

Theorem

$(\bar{h}, \bar{\sigma}, H_{\bar{h},\sigma}) \in X(e_0;\mathbf{B})$ *minimizer.*

Then $\bar{h}$ has at most finitely many cusp points and vertical cracks, its graph is of class C^1 away from this finite set, and of class $C^{1,\alpha}$, $\alpha \in (0, \frac{1}{2})$ away from this finite set and off the substrate.

Major difficulty: to show that the *volume constraint can be replaced by a volume penalization*. Dislocation-free case – **straightforward truncation argument**. This fails here because dislocations cannot be removed in this way, they act as obstacles

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Migration to the Substrate

Analytical validation of experimental evidence:
after nucleation, dislocations lie at the bottom !

Theorem

Assume $\mathbf{B} \neq \emptyset$, $d > 2r_0 b$.

There exist $\bar{e} > 0$ *and* $\bar{\gamma} > 0$ *such that whenever* $|e_0| > \bar{e}$, $\gamma > \bar{\gamma}$, *and* $e_0(\mathbf{b}_j \cdot \mathbf{e}_1) > 0$ *for all* $\mathbf{b}_j \in \mathbf{B}$,

then any minimizer $(\bar{h}, \bar{\sigma}, \bar{H})$ *has all dislocations lying at the bottom of* Ω_h *: the centers* z_i *are of the form* $z_i = (x_i, r_0)$.

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When is Energetically Favorable to Create Dislocations?

Assume that the energy cost of a new dislocation is proportional to the square of the norm of the corresponding Burgers vector (*Nabarro, Theory of Crystal Dislocations, 1967*)

New variational problem:

$$\text{minimize} \quad F(h, \sigma, H) + N(\sigma)$$

We identify a range of parameters for which all

global minimizers have nontrivial dislocation measures.

Theorem

Assume that there exists $\mathbf{b} \in \mathcal{B}^o$ *such that* $\mathbf{b} \cdot \mathbf{e}_1 \neq 0$, *and let* $d > 2r_0 b$.

Then there exists $\bar{\gamma} > 0$ *such that whenever* $|e_0| > \bar{e}$, *and* $\gamma > \bar{\gamma}$,

then any minimizer $(\bar{h}, \bar{\sigma}, \bar{H})$ *has nontrivial dislocations, i.e.,* $\bar{\sigma} \neq 0$.

Analysis

Open Problems and Future Directions

- What if the substrate is exposed, i.e., with initial profile $h_0 \geq 0$ but $|\{h_0 = 0\}| > 0$
- Uniqueness in three-dimensions
- More general global existence results
- The non-graph case
- The convex case, without curvature regularization
- More general $H^{-\alpha}$-gradient flows: the nonlocal Mullins-Sekerka law
- Dislocations!

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