Quantum Dots and Dislocations: Dynamics of Materials Defects
most in collaboration with N. Fusco, G. Leoni and M. Morini

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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 thickness
- lattice misfits between substrate and film induce strains in the film
- Complete relaxation to bulk equilibrium $\Rightarrow$ crystalline structure would be discontinuous at the interface
- Strain $\Rightarrow$ 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 (quantum 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.
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

\[ F(h,u) := \int_{\Omega_h} W(E(u)) \, dx \, dy + \int_{\Gamma_h} \psi(\nu) \, d\sigma \]

\[ E(u) = \frac{1}{2} (\nabla u + \nabla^T u) \quad \text{... strain} \]

\[ W(E) = \frac{1}{2} E \cdot \mathbb{C} E \quad \text{... energy density} \]

\[ \mathbb{C} \quad \text{... positive definite fourth-order tensor} \]

\[ \psi = \ldots \text{(anisotropic) surface energy density} \]

\[ u(x,0) = e_0(x,0), \quad \nabla u(\cdot, t) \quad \text{... Q-periodic} \]
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- \( W(E) = \frac{1}{2} E \cdot C \cdot E \) ... energy density
- \( C \) ... positive definite fourth-order tensor
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Substrate

\[ 0 \quad \Gamma_h \quad \Omega_h \quad b \]
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\[ \inf \{ F(h, u) : (h, u) \text{ admissible}, \, |\Omega_h| = d \} \]
$$F(h, u) := \int_{\Omega_h} W(E(u)) \, dx \, dy + \int_{\Gamma_h} \psi(\nu) \, d\sigma$$

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)

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

$$e_0 > 0$$

$$i$$ the unit vector along the $$x$$ direction

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

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

$$C$$ . . . positive definite fourth-order tensor

film and substrate have similar material properties, share the same homogeneous elasticity tensor $$C$$
\[ \psi(y) := \begin{cases} \gamma_{\text{film}} & \text{if } y > 0, \\ \gamma_{\text{sub}} & \text{if } y = 0. \end{cases} \]

**Total energy of the system:**

\[
F(u, \Omega_h) := \int_{\Omega_h} W(E(u)(x,y) - E_0(y)) \, dx + \int_{\Gamma_h} \psi(y) \, d\mathcal{H}^1(x),
\]

\[ \Gamma_h := \partial \Omega_h \cap ((0, b) \times \mathbb{R}) \ldots \text{free surface of the film} \]
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 $\delta$ (“smearing parameter”)

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

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

\[
f(0) = 0, \quad \lim_{y \to -\infty} f(y) = -1, \quad \lim_{y \to \infty} f(y) = 1
\]
smooth transition – total energy of the system:

\[ F_\delta(u, \Omega_h) := \int_{\Omega_h} W(E(u)(x, y) - E_\delta(y)) \, dx + \int_{\Gamma_h} \psi_\delta(y) \, d\mathcal{H}^1(x) \]

Two regimes:

\[
\begin{cases}
\gamma_{\text{film}} \geq \gamma_{\text{sub}} \\
\gamma_{\text{film}} < \gamma_{\text{sub}}
\end{cases}
\]
asymptotics as $\delta \to 0^+$

- $\gamma_{\text{film}} < \gamma_{\text{sub}}$
  
  relaxed surface energy density is no longer discontinuous: it is constantly equal to $\gamma_{\text{film}}$... WETTING!

- more favorable to cover the substrate with an infinitesimal layer of film atoms (and pay surface energy with density $\gamma_{\text{film}}$) rather than to leave any part of the substrate exposed (and pay surface energy with density $\gamma_{\text{sub}}$)

- wetting regime: regularity of local minimizers $(u, \Omega)$ of the limiting functional $F_\infty$ under a volume constraint
Wetting, etc.

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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$_{0.4}$.

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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 $u$ near the boundary $\Rightarrow C^{1,\alpha}$ regularity of $h$ and $\nabla u$; bootstrap

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Linearly Isotropic Elastic Materials

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

\( \lambda \) and \( \mu \) are the (constant) Lamé moduli

\[ \mu > 0, \quad \mu + \lambda > 0. \]

Euler-Lagrange system of equations associated to \( W \)

\[ \mu \Delta u + (\lambda + \mu) \nabla (\text{div } u) = 0 \quad \text{in } \Omega. \]
Regularity of $\Gamma$: No Corners

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

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

**Theorem**

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

If $z_0 = (x_0, 0) \in \Gamma \setminus \Gamma_{\text{sing}}$ then $h'(x_0) = 0$. 
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If $z_0 = (x_0, 0) \in \Gamma \setminus \Gamma_{\text{sing}}$ then $h'(x_0) = 0$. 
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:**

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

height profile $u$, $\text{supp}(u) = [0, L]$

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

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

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**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.
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 $d \in (0, \overline{d})$
The presence of the island, where that type is stable; and the half-pyramid shape is independent of size. We show the largest stable island of each type, the shape varies only modestly over the entire range of volume increasing from bottom to top. We show the largest stable island of increasing volume from bottom to top. We show the largest stable island of increasing volume from bottom to top.

**Figure:** Shape transitions with increasing volume at miscut angle $3^\circ$. Numerical simulation. Courtesy of B. Spencer and J. Tersoff, *Appl. Phys. Lett.* 96, 073114 (2010).
Einstein-Nernst Law: surface flux of atoms $\propto \nabla_{\Gamma} \mu$

$\mu =$ chemical potential $\Rightarrow V = c \times \Delta_{\Gamma(t)} \mu$

Laplace-Beltrami operator (volume preserving)

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

anisotropic curvature

$V = \Delta_{\Gamma} \left( \text{div}_{\Gamma} D\psi(\nu) + W(E(u)) \right)$
**Surface Diffusion in Epitaxially Strained Solids**

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

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\( \lambda \) is anisotropic curvature

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Highly Anisotropic Surface Energies

For highly anisotropic $\psi$ 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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$\Downarrow$

$$V = \Delta_\Gamma \left[ \text{div}_\Gamma(D\psi(\nu)) + W(E(u)) - \varepsilon \left( \Delta_\Gamma(|H|^{p-2} H) - |H|^{p-2} H \left( \kappa_1^2 + \kappa_2^2 - \frac{1}{p} H^2 \right) \right) \right]$$
Highly Anisotropic Surface Energies in 2D

Regularized energy:

\[ F(h, u) := \int_{\Omega_h} W(E(u)) \, dx \, dy + \int_{\Gamma_h} (\psi(\nu) + \frac{\varepsilon}{2}k^2) \, d\mathcal{H}^1 \]

Why here \( p > 2 \): technical \ldots in two dimensions, the Sobolev space \( W^{2,p} \) embeds into \( C^{1,(p-2)/p} \) if \( p > 2 \).
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\[ V = \left( \text{div}_\sigma D\psi(\nu) + W(E(u)) - \varepsilon(k_{\sigma\sigma} + \frac{1}{2} k^3) \right)_{\sigma\sigma} \]

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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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The Evolution Law

- Curvature dependent energies $\sim$ Herring (1951)
- 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 $h : \mathbb{R}^2 \times [0, T_0] \to (0, +\infty)$ s.t.

$$
\begin{align*}
\frac{1}{J} \frac{\partial h}{\partial t} &= \Delta \Gamma \left[ \text{div}_\Gamma (D\psi (\nu)) + W (E (u)) \\
&\quad - \varepsilon \left( \Delta \Gamma (|H|^{p-2} H) - |H|^{p-2} H \left( \kappa_1^2 + \kappa_2^2 - \frac{1}{p} H^2 \right) \right) \right], \quad \text{in } \mathbb{R}^2 \times (0, T_0) \\
\text{div} \mathcal{C}E (u) &= 0 \quad \text{in } \Omega_h \\
\mathcal{C}E (u)[\nu] &= 0 \quad \text{on } \Gamma_h, \quad u (x, 0, t) = e_0 (x, 0) \\
h (\cdot, t) \text{ and } Du (\cdot, t) \quad &\text{are } Q\text{-periodic} \\
h (\cdot, 0) = h_0
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$$

Here $J := \sqrt{1 + |Dh|^2}$
The Evolution Law

- Curvature dependent energies \(\sim\) Herring (1951)
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Given \(Q\), find \(h: \mathbb{R}^2 \times [0, T_0] \rightarrow (0, +\infty)\) s.t.

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Some Related Results

- Siegel, Miksis, Voorhees (2004): numerical experiments in the case of evolving curves

- 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

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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

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

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

$$g_{\Omega_h}(V_1, V_2) := \int_{\Gamma_h} \nabla_{\Gamma_h} w_1 \nabla_{\Gamma_h} w_2 \, d\sigma$$

for all $V_1, V_2 \in T_{\Omega_h}M$, where $w_i, i = 1, 2$, is the solution to

$$\begin{cases} -\Delta_{\Gamma_h} w_i = V_i & \text{on } \Gamma_h, \\ w_i \text{ is } Q\text{-periodic,} \\ \int_{\Gamma_h} w_i \, d\sigma = 0. \end{cases}$$
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Consider the reduced functional

\[ F(h, u) \sim \overline{F}(\Omega_h) := F(h, u_h) \]

where \( u_h \) is the elastic equilibrium in \( \Omega_h \).

The evolution law is formally equivalent to

\[ g_{\Omega_h(t)}(V, \tilde{V}) = -\partial \overline{F}(\Omega_{h(t)})[\tilde{V}] \quad \text{for all } \tilde{V} \in T_{\Omega_{h(t)}} \mathcal{M}, \]

where \( \partial \overline{F}(\Omega_{h(t)})[\tilde{V}] \) = first variation of \( \overline{F} \) at \( \Omega_{h(t)} \) in the direction \( \tilde{V} \).

First observed by Cahn & Taylor (1994) in the context of surface diffusion.
The Gradient Flow Structure, cont.

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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 $\sim$ De Giorgi’s minimizing movements
- In the context of geometric flows $\sim$ 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

\[
\min_{(h, u) \text{ admissible}} F(h, u) + \frac{1}{2\tau} \int_{\Gamma_{h_{i-1}}} |D\Gamma_{h_{i-1}} w_h|^2 d\mathcal{H}^2
\]

where

\[
\Delta \Gamma_{h_{i-1}} w_h = h - h_{i-1} \sqrt{1 + |Dh_{i-1}|^2} =: V_{\Omega h},
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with $\|Dh\|_{\infty} \leq C$. 

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

where

$$\begin{cases}
\Delta_{\Gamma_{h_{i-1}}} w_h = \frac{h - h_{i-1}}{\sqrt{1 + |Dh_{i-1}|^2}} =: V_{\Omega h}, \\
\int_{\Gamma_{h_{i-1}}} w_h d\mathcal{H}^2 = 0.
\end{cases}$$

$$\frac{1}{2\tau} \int_{\Gamma_{h_{i-1}}} |D_{\Gamma_{h_{i-1}}} w_h|^2 d\mathcal{H}^2 \sim \|h - h_{i-1}\|^2_{H^{-1}(\Gamma_{h_{i-1}})}$$
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The Discrete Euler-Lagrange Equation

The Euler-Lagrange equation of the incremental problem is

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

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}} \left[ \text{div}_{\Gamma_{h_i}} (D\psi(\nu)) + W(E(u_i)) \\
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this is a discrete version of the continuous evolution law
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this is a discrete version of the continuous evolution law
Estimates

\[ h_N(\cdot, t) = h_{i-1} + \frac{t-(i-1)\tau}{\tau}(h_i - h_{i-1}) \quad \text{if } (i-1)\tau \leq t \leq i\tau \]

Basic energy estimate:

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

\[
\sum_{i=1}^{N} \frac{1}{2\tau} \|h_i - h_{i-1}\|_{H^{-1}}^2 \leq \sum_{i=1}^{N} (F(h_{i-1}, u_{i-1}) - F(h_{i}, u_{i})) \leq CF(h_0, u_0)
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\[ \{h_N\} \text{ is bounded in } H^1(0, T; H^{-1}) \]
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\[ \downarrow \]

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Local in Time Existence of Weak Solutions

- Previous estimates + interpolation inequalities + higher regularity + compactness argument \( \leadsto h_N \rightarrow h \) (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) \[ \text{div}_\Gamma(D \psi(\nu)) + W(E(u)) - \varepsilon \left( \Delta_\Gamma(|H|^{p-2}H) - \frac{1}{p} |H|^p H + |H|^{p-2}H|B|^2 \right) \in L^2(0, T_0; H^1_\#(Q)), \]

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

\[ \frac{1}{J} \frac{\partial h}{\partial t} = \Delta_\Gamma \left[ \text{div}_\Gamma(D \psi(\nu)) + W(E(u)) \\ - \varepsilon \left( \Delta_\Gamma(|H|^{p-2}H) - |H|^{p-2}H \left( \kappa_1^2 + \kappa_2^2 - \frac{1}{p} H^2 \right) \right) \right] \] in \( H^{-1}_\#(Q) \).
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(ii) for a.e. \( t \in (0, T_0) \)

\[
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\]
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

\[
\frac{1}{J} \frac{\partial h}{\partial t} = \Delta \Gamma \left[ \text{div}_\Gamma (D \psi (\nu)) + W(E(u)) \right.
\]

\[-\varepsilon \left( \Delta \Gamma (|H|^{p-2}H) - |H|^{p-2}H \left( \kappa_1^2 + \kappa_2^2 - \frac{1}{p} H^2 \right) \right) \right]
\]

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.
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) $h(\cdot, t) \rightarrow d$ in $W^{2,p}$ as $t \rightarrow +\infty$. 
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 \( W_\psi \) 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 \Rightarrow \quad \|h(t) - d\|_{W^{2,p}} \leq \sigma \quad \text{for all } t > 0.
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\[
\int_Q h_0 = d, \quad \|h_0 - d\|_{W^{2,p}} \leq \delta(\sigma) \quad \implies \quad \|h(t) - d\|_{W^{2,p}} \leq \sigma \text{ for all } t > 0.
\]
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

• dislocations migrate to the film/substrate interface and the film surface relaxes towards a planar-like morphology.
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Microscopic Level

- Perfect crystals

Figure: Courtesy of James Hedberg
Microscopic Level

- Defects in crystalline materials

Figure: Courtesy of Helmut Föll
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)
- Dislocation line

Figure: Courtesy of J. W. Morris, Jr
Microscopic Level

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Microscopic Level

- Screw dislocations
- Burgers vector

Figure: Courtesy of Helmut Föll
Microscopic Level

- Screw dislocations
- Burgers vector

Figure: Courtesy of Helmut Föll
Epitaxy and Dislocations: The Model

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

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

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

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

... now with the presence of isolated misfit dislocations in the film
Epitaxy and Dislocations: The Model

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Epitaxy and Dislocations: The Model With Dislocations

System of Dislocations located at $z_1, \ldots, z_k$ with Burgers Vectors $b_1, \ldots, b_k$

\[ \text{curl } H = \sum_{i=1}^{k} b_i \delta_{z_i} \]

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 $\sigma := \sum_{i=1}^{k} b_i \delta_{z_i}$ through a convolution procedure
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Epitaxy and Dislocations: More on the Model With Dislocations

\[ \nabla \times H = \sigma \ast \rho_{r_0} \cdot \quad \rho_{r_0} := \left( \frac{1}{r_0^2} \right) \rho(\cdot / r_0) \quad \text{standard mollifier} \]

Total energy associated with a profile \( h \), a dislocation measure \( \sigma \) and a strain field \( H \)

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

What we ask : Assume that a finite number \( k \) of dislocations, with given Burgers vectors \( B := \{ b_1, \ldots, b_k \} \subset \mathbb{R}^2 \), are already present in the film
curl $H = \sigma \ast \rho_{r_0} \cdot \rho_{r_0} := (1/r_0^2)\rho(\cdot/r_0)$ standard mollifier

Total energy associated with a profile $h$, a dislocation measure $\sigma$ and a strain field $H$

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

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

### Theorem

The minimization problem

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

admits a solution.

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

### Theorem

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

---

Irene Fonseca (Department of Mathematical Sciences Center for Nonlinear Analysis Carnegie Mellon University Supported by the National Science Foundation (NSF))

Epitaxy and Dislocations

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Migration to the Substrate

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

**Theorem**

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

There exist $\bar{e} > 0$ and $\bar{\gamma} > 0$ such that whenever $|e_0| > \bar{e}$, $\gamma > \bar{\gamma}$, and $e_0(b_j \cdot e_1) > 0$ for all $b_j \in B$,

then any minimizer $(\bar{h}, \bar{\sigma}, \bar{H})$ has all dislocations lying at the bottom of $\Omega_h$: the centers $z_i$ are of the form $z_i = (x_i, r_0)$. 
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 $b \in B^o$ such that $b \cdot e_1 \neq 0$, and let $d > 2r_0b$.

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., $\bar{\sigma} \neq 0$. 

[Irene Fonseca (Department of Mathematical Sciences Center for Nonlinear Analysis Carnegie Mellon University Supported by the National Science Foundation (NSF))](#)
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

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- 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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