Uniform distribution of dislocations at semi-coherent interfaces

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Joint work with

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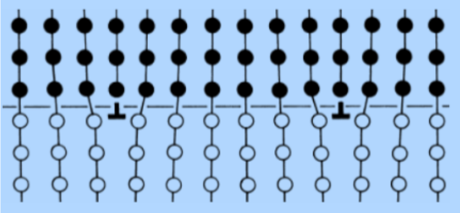
Semi-coherent interfaces

Semicoherent interfaces $\rightsquigarrow$ interfaces between two crystals with (slightly) different lattice spacing

In the vicinity of the interface there are many atoms having the “wrong” coordination number: **edge dislocations**

Energy: $E^{el} + E^{inter}(+E^{core})$



- Dislocations release bulk elastic energy
- A periodic distribution of dislocations induces a periodic displacement around the interface

Classical literature

Assume:

- **Periodic distribution of dislocations**
- Sinusoidal interfacial energy (zero if two atoms are vertically aligned, maximal on the dislocation cores) and linear elasticity

Then, one can compute:

- The optimal transition profile for the displacements at interface: concentrated around the cores
- The effective surface energy of the interface

F. R. N. Nabarro. Dislocations in a simple cubic lattice. *Proc. Phys. Soc.*, 1947

R. Peierls. The size of a dislocation. *Proc. Phys. Soc.*, 1940

J.H. Van Der Merwe. On the stresses and energies associated with inter-crystalline boundaries. *Proc. Phys. Soc. A*, 1950

Question: Rigorous proof of the periodic distribution of dislocations

The variational model

Details and assumptions of the model:

(A1) The underlying lattice is rigid

Main variable: $u : \mathbb{R} \to \mathbb{R}$ is the displacement at the interface

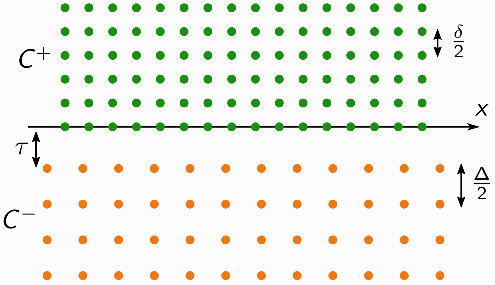
Notice: We have perfect matching if $u' \equiv \lambda$ for some (specific) $0 < \lambda \ll 1$. The dislocation cores are regions where $u' \approx -\frac{1}{2}$.

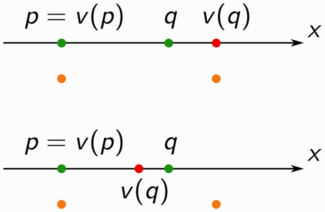
(A2) We assume either perfect matching or dislocation cores:

- **Perfect matching:** where $u' = \lambda$
- **Dislocation cores:** Intervals with length equal to δ, of the order of the lattice spacing, where the profile of u is rigid
  For simplicity $u' \equiv -\Lambda \approx -\frac{1}{2}$ on such dislocation cores

(A3) Elastic energy $\mapsto$ Dirichlet energy (unphysical!)

The discrete picture





Left: reference configuration

Top Right: Purely elastic displacement $u = \frac{(\Delta-\delta)}{2}$, $u' = \frac{\Delta}{\delta} - 1 =: \lambda$

Bottom Right: Edge dislocation, $u = \frac{\Delta}{4} - \frac{\delta}{2}$, $u' = \frac{\Delta}{2\delta} - 1 \approx -\frac{1}{2}$

Piece-wise affine interpolation... $u' \in \left\{\lambda := \frac{\Delta}{\delta} - 1, -\Lambda := \frac{\Delta}{2\delta} - 1\right\}$

The variational problem

Dirichlet energy of $U : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R} \rightsquigarrow \| Tr(U)\|^2_{\dot{H}^{1/2}}$

Infinite surface energy. We consider a finite interface of size $l > 0$

Admissible displacements: $u : [0, l] \to \mathbb{R}$ with $u' \in \{\lambda, -\Lambda\}$ and with $\{u' = -\Lambda\}$ given by union of disjoint segments of size δ

The energy functional:

$$E^l(u) := \|u\|^2_{\dot{H}^{1/2}} = \int_0^l \int_0^l \frac{|u(x) - u(y)|^2}{|x - y|^2} \, dx \, dy$$

Questions:

- Γ-limit as $l \to +\infty$
- Asymptotic behaviour of minimizers; uniform distribution of dislocations

Energy scaling

The energy scales like the length of the interface

Theorem

There exists $0 < c_\infty < \infty$ *such that*

$$\min_u \frac{1}{l} \int_0^l \int_0^l \frac{|u(x) - u(y)|^2}{|x - y|^2} \, dxdy \to c_\infty$$

Proof: Let E_l be the minimal energy on $[0, l]$. Then $E_{\frac{l}{2}} \leq \frac{1}{2} E_l$

$\frac{1}{nl} E_{nl}$ is monotone $\rightsquigarrow$ $\frac{1}{l} E_l$ is almost monotone

Surface energy density: c_∞ is the minimal energy density induced by dislocations, whose presence is enforced by the lattice misfit

Uniform distribution of dislocations

Scaled displacement: Let $w_l(x) := \frac{u(lx)}{\sqrt{l}}$

$$\frac{1}{l} E^l(u_l) = \|w_l\|^2_{\dot{H}^{1/2}([01])} =: F^l(w_l)$$

Scaled dislocations: Given w_l we plug a Dirac mass in the center of each interval in $[0,1]$ where $w_l' = -\Lambda\sqrt{l}$, obtaining an **empirical measure** μ_l on $[0,1]$

Theorem

Let w_l be minimizers of F^l. Then (up to an additive constant) $w_l \rightharpoonup 0$ in $H^{\frac{1}{2}}([0,1])$.

As a consequence, as $l \to +\infty$

$$\frac{1}{l}\mu_l \overset{*}{\rightharpoonup} \frac{\Lambda}{\delta(\Lambda+\lambda)}.$$

Proof: $\int_I \int_J \frac{|w_l(x)-w_l(y)|^2}{|x-y|^2}\, dxdy \to 0 \quad \forall\, I, J \subset [0,1] :\ I \cap J = \emptyset.$

Γ-convergence

Theorem (Γ-convergence)

As $l \to +\infty$, the functionals F^l Γ-converge with respect to the weak topology of $H^{\frac{1}{2}}(0,1)$ to the functional

$$F^\infty(w) := c_\infty + \int_0^1 \int_0^1 \frac{|w(x) - w(y)|^2}{|x-y|^2} \, dxdy$$

- c_∞ is the surface energy induced by uniformly distributed dislocations
- $\|w\|_{\dot{H}^{\frac{1}{2}}}$ is the far field elastic energy, induced by further (possibly not uniformly distributed) dislocations

Proof of Γ-liminf:

Divide $[0,1]$ in N equal intervals I_i

- **Self interactions:** We have

$$\frac{1}{N} c_\infty \leq \liminf \int_{I_i} \int_{I_i} \frac{|w_I(x) - w_I(y)|^2}{|x-y|^2} \, dxdy$$

Summing over i we get the lower bound with c_∞

- **Mutual interactions:** By l.s.c.

$$\int_{I_i} \int_{I_j} \frac{|w(x) - w(y)|^2}{|x-y|^2} \, dxdy \leq \liminf \int_{I_i} \int_{I_j} \frac{|w_I(x) - w_I(y)|^2}{|x-y|^2} \, dxdy$$

as $N \to +\infty$ the sum of the mutual interactions tends to $\|w\|^2_{\dot{H}^{\frac{1}{2}}}$

Proof of Γ-limsup:

Density argument: Assume w piece-wise affine. $w' = \sum_{h=1}^{N} \lambda_h \chi_{I_h}$

Construction:

- **Misfit dislocations:** Plug the dislocations induced by the misfit. These necessary dislocations are of order l, induce a zero-average oscillating displacement and c_∞ energy
- **Further dislocations:** On each interval I_h either add or remove some dislocations (uniformly), according with the sign of $w' = \lambda_h$ These further dislocations are of order $\lambda_h \sqrt{l}$, they induce the macroscopic strain w, and energy $\|w\|^2_{\dot{H}^{\frac{1}{2}}}$.

Additive decomposition of the energy: Show that in the limit these two contributions in the energy become additive

Periodic distribution of dislocations

Are dislocations evenly spaced in the limit as $l \to \infty$?

Partial answer: Yes, for a simplified model:

- **Semi-coherent $\mapsto$ coherent:** Finite number of dislocations
- **Periodic boundary conditions:** The model is set on S^1
- **Minimal distance between dislocations proportional to l:** Single dislocations on S^1

Reduced energy functional: In this simplified setting the energy can be written as a function of the dislocation points:

$$E(x_i, \dots, x_n) \approx -\sum_{i \neq j} \log(|x_i - x_j|)$$

It is a convex function of the mutual distances between dislocations.

Convexity $\mapsto$ equal distances

Comparison with phase-field models

Modica-Mortola approach: Set $f(x) := u(x) - \lambda x$

$$E_\varepsilon(f) := \varepsilon \|f(x) + \lambda x\|^2_{\dot{H}^{\frac{1}{2}}} + \frac{1}{\varepsilon} \int \mathrm{dist}^2\Big(f(x), \frac{\Delta}{2}\mathbb{Z}\Big)\, dx$$

Question: Asymptotic analysis as $\varepsilon \approx \Delta \to 0$ (and maybe $\lambda \to 0$)?

Nabarro, Peierls, Van Der Merwe: Optimal profile.

G. Alberti, G. Bouchitté, and P. Seppecher: $\Delta = 1$, $\lambda = 0$.

Ohta-Kawasaki approach:

$$OK_{\varepsilon, H^{-1}}(v) := \|v\|^2_{H^{-1}} + \varepsilon^2 \|v'\|^2_2 + \|v^2 - 1\|^2_2$$

S. Müller. Singular perturbations as a selection criterion for periodic minimizing sequences. *Calc. Var.*, 1993.

Energy functional: $\|u\|^2_{H^{\frac{1}{2}}} + \varepsilon^2 \|u''\|^2_2 + \|\mathrm{dist}(u', \{\lambda, -\Lambda\})\|^2_2$

Setting $u' = v \mapsto OK_{\varepsilon, H^{-\frac{1}{2}}}(v) := \|v\|^2_{H^{-\frac{1}{2}}} + \varepsilon^2 \|v'\|^2_2 + \|\mathrm{dist}(v, \{\lambda, -\Lambda\})\|^2_2$

Heterogeneous lattices

Misfit dislocations: Heterogeneous lattices, epitaxial growth:
The total energy accounts also the surface energy induced by the exterior boundary of the overlayer

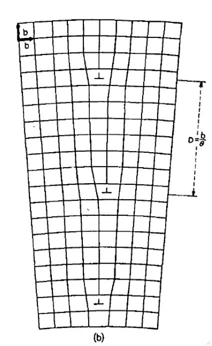
I. Fonseca, N. Fusco, G. Leoni, and M. Morini. A model for dislocations in epitaxially strained elastic films. *J. Math. Pures Appl.*, 2018.

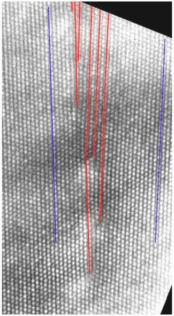
P.B. Hirsch. Nucleation and propagation of misfits dislocations in strained epitaxial layer systems. In *Proceedings of the Second International Conference Schwäbisch Hall, Fed. Rep. of Germany* (1990).

Purely discrete models:

G. Lazzaroni, M. Palombaro, and A. Schlömerkemper. A discrete to continuum analysis of dislocations in nanowires heterostructures. *Communications in Mathematical Sciences*, **13** (2015).

Grain boundaries





Tilt boundaries: misfit between crystal lattices are described by rotations rather than dilations.

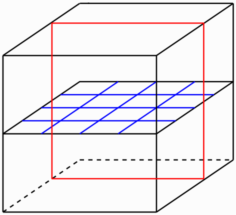
W. T. Read and W. Shockley. Dislocation models of crystal grain boundaries. *Phys. Rev.*, **78** (1950).

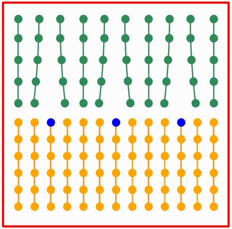
G. Lauteri and S. Luckhaus. An energy estimate for dislocation configurations and the emergence of cosserat-type structures in metal plasticity. Preprint 2016.

S. Fanzon, M. Palombaro, and M. Ponsiglione. Derivation of linearised polycrystals from a two-dimensional system of edge dislocations. *SIMA*, 2019.

2D semicoherent interfaces

Van der Merwe: "...because the equations are linear to the degree of approximation used, solutions may be superposed and the following treatment easily extended to cover the case of misfit in both the x and y directions."





S. Fanzon, M. Palombaro, M. Ponsiglione: A Variational Model for Dislocations at Semi-coherent Interfaces. *J. Nonlinar Sci.* **27**, 2017.

Question: Square vs Hexagonal lattice? Variational/Kinematic principles?

M Koslowski and M Ortiz : A multi-phase field model of planar dislocation networks *Modelling Simul. Mater. Sci. Eng.* **12**, 2004.

T. Hales: The honeycomb conjecture. *Discrete Comput Geom* **25** (2001).