A variational model for dislocations at semi-coherent interfaces

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in collaboration with

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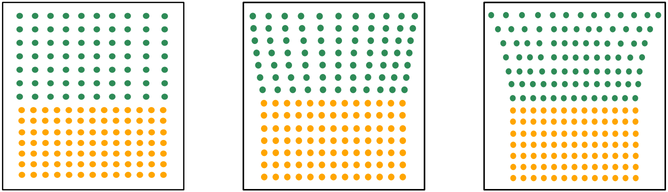
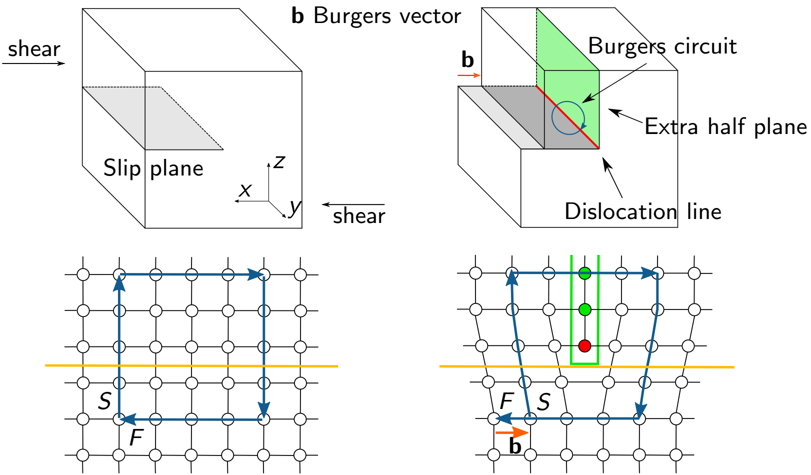


S. Fanzon, M. Palombaro and M. Ponsiglione. A variational model for dislocations at semi-coherent interfaces. *Journal of Nonlinear Science* (To appear).

Nucleation of an edge dislocation

Dislocations: topological defects in the otherwise periodic structure of a crystal.
Edge dislocation: Burgers vector is orthogonal to dislocation line.



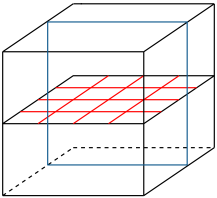
Semi-coherent interfaces

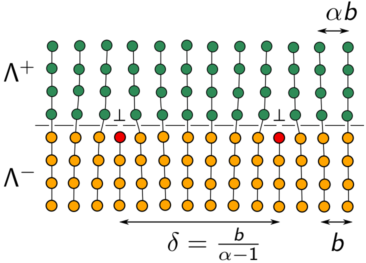
Semi-coherent interface: two crystalline materials joined at a flat interface:

- **Underlayer:** cubic lattice Λ^- with spacing $b > 0$,
- **Overlayer:** lattice $\Lambda^+ = \alpha\Lambda^-$, lying on top of Λ^-, with $\alpha \approx 1$ dilation.

Experimentally observed phenomena:

- interface mismatch accommodated by two non-parallel sets of edge dislocations with spacing $\delta = \frac{b}{\alpha - 1}$
- far field stress is completely relieved





D.A. Porter, K.E. Easterling. Phase transformations in metals and alloys. CRC Press (2009)

G. Gottstein. Physical foundations of materials science. Springer (2013)

Our goal

$\alpha > 1$ is the dilation and R is the size of the interface.

Goal: define a continuum model that captures the main features of the above phenomena:

- $\exists$ a threshold R^* such that nucleation of dislocations is energetically more favorable for $R > R^*$
- as $R \to \infty$ the far field stress is relieved
- the dislocation spacing tends to $\delta = \dfrac{b}{\alpha - 1}$

Plan:

- start from the analysis of a semi-discrete model where dislocations are line defects
- the analysis will motivate the definition of a simplified (dislocation density) continuum model.

Semi-discrete line defect model

The body: $\Omega_R := \Omega_R^- \cup S_R \cup \Omega_R^+$ with $R > 0$,

- Ω_R^+ overlayer (equilibrium αI)
- Ω_R^- underlayer (in equilibrium and rigid)

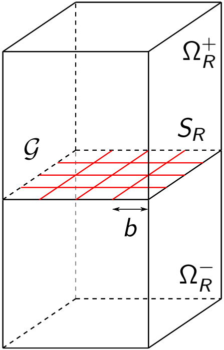
Dislocation curves: relatively closed curves on $\mathcal{G} \subset S_R$. $\mathcal{G} := (b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z})$ with b lattice spacing of Ω_R.

Admissible dislocations: $(\Gamma, \mathbf{B}) \in \mathcal{AD}$ if $\Gamma = \{\gamma_i\}$, $\mathbf{B} = \{\mathbf{b}_i\}$ finite collection of $\gamma_i \subset \mathcal{G}$ and $\mathbf{b}_i \in b(\mathbb{Z} \oplus \mathbb{Z})$ corresponding Burgers vector.

Admissible strains: fix $1 < p < 2$. $F \in L^p(\Omega_R; \mathbb{M}^{3\times 3})$ s.t.

$$F = I \text{ in } \Omega_R^- \quad \text{and} \quad \operatorname{curl} F = -\mathbf{b} \otimes \dot\gamma \, d\mathcal{H}^1 \llcorner \Gamma$$

is an admissible strain for $(\Gamma, \mathbf{B})$. We write $F \in AS(\Gamma, \mathbf{B})$.



Energy density: $W(F) \sim \operatorname{dist}(F, \alpha SO(3))^2 \wedge (|F|^p + 1)$

Dislocation Energy: he energy induced by the dislocation $(\Gamma, \mathbf{B})$ is

$$E_{\alpha,R}(\Gamma, \mathbf{B}) := \inf \left\{ \int_{\Omega_R^+} W(F(x))\, dx : F \in \mathcal{AS}(\Gamma, \mathbf{B}) \right\}$$

Energies induced by the misfit:

- $E_{\alpha,R}(\emptyset) := \inf \left\{ \int_{\Omega_R^+} W(F(x))\, dx : \ \operatorname{curl} F = 0 \right\}$ (Elastic energy)
- $E_{\alpha,R} := \min \{ E_{\alpha,R}(\Gamma, \mathbf{B}) : \ (\Gamma, \mathbf{B}) \in \mathcal{AD} \}$ (Plastic energy)

Theorem (F., Palombaro, Ponsiglione (2015))

The dislocation-free elastic energy scales like R^3*: we have* $E_{\alpha,1}(\emptyset) > 0$ *and*

$$E_{\alpha,R}(\emptyset) = R^3\, E_{\alpha,1}(\emptyset)\,.$$

The minimal energy induced by the lattice misfit scales like R^2*: there exists* $0 < E_\alpha < +\infty$ *such that*

$$\lim_{R \to +\infty} \frac{E_{\alpha,R}}{R^2} = E_\alpha .$$

In particular, for large R *dislocations are energetically favorable.*

S. Müller and M. Palombaro (2008) - G. Lazzaroni, M. Palombaro and A. Schlömerkemper (2015)

Upper bound construction

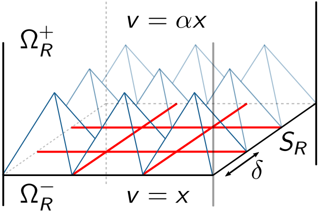
Construction: define a square array of edge dislocations with spacing $\delta := \dfrac{b}{\alpha - 1}$

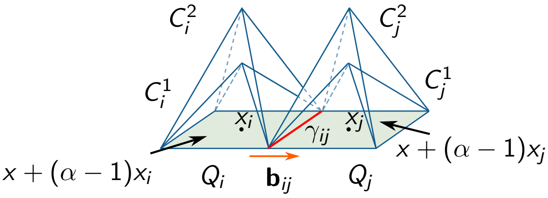
1. Divide S_R into $(R/\delta)^2$ squares of side δ
2. Above Q_i define pyramids C_i^1 (height $\delta/2$) and C_i^2 (height δ)
3. Deformation v defined as in the pictures.

Induced dislocations: if Q_i and Q_j adjacent then

- $\gamma_{ij} := Q_i \cap Q_j$ admissible dislocation curve ($\delta = nb$ as $\alpha = 1 + 1/n$)
- $\mathbf{b}_{ij} := (\alpha - 1)(x_j - x_i) = \pm b\,\mathbf{e}_s$ Burgers vector (for some $s = 1, 2$).

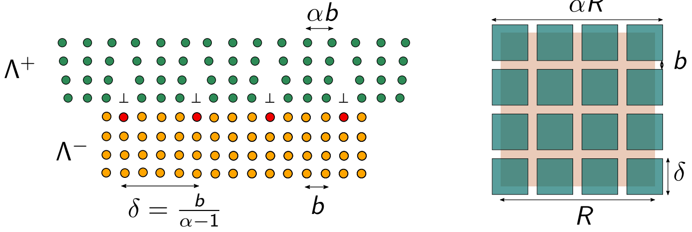
Energy: in every pyramid it is bounded by $c = c(\alpha, b, p)$. Therefore $E_{\alpha,R} \leq c\dfrac{R^2}{\delta^2}$ since $W(\alpha I) = 0$.





Some comments on the semi-discrete model

Deformed configuration: $v(S_R)$ with v as in the upper bound construction



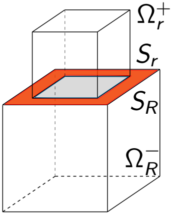
Limitations of the considered model:

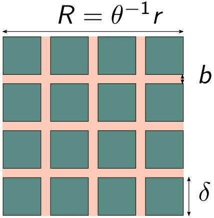
1. $v(S_R)$ does not match $S_R \implies$ not appropriate for semi-coherent interfaces;
2. v induces the expected dislocation geometry with spacing $\frac{b}{\alpha-1}$. However its energy is only optimal in the scaling.

What we do now:

1. consider a smaller overlayer $\Omega^+_{\theta R}$ with $\theta \in [\alpha^{-1}, 1]$ and enforce a perfect match between the underlayer and the deformed overlayer;
2. introduce a simplified continuum (dislocation density) model to better describe true minimizers.

Hypothesis for the continuum model





The body: set $r := \theta R$ with $\theta \in [\alpha^{-1}, 1]$ and $\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+$.
Upper bound construction: with $\theta = \alpha^{-1}$ and $\delta = \frac{b}{\theta^{-1}-1} \implies$ perfect match

$$\text{Dislocation Length} \approx \frac{1}{b} \text{Area Gap}$$

We proved that as $r \to \infty$

$$E_{\alpha,r} \approx r^2 E_\alpha = \sigma \,\text{Area Gap} \implies E_{\alpha,r} \propto \text{Dislocation Length}$$

Hypothesis for continuum model: dislocation energy assumed proportional to the total dislocation length. We then optimize over θ.

The body: $\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+$. Here $r := \theta R$ with $\theta \in [\alpha^{-1}, 1]$.

Admissible deformations: $v \in W^{1,2}(\Omega_r^+; \mathbb{R}^3)$ enforcing $v(x) = x/\theta$ on $S_r \implies v(S_r) = S_R$ (interface match).

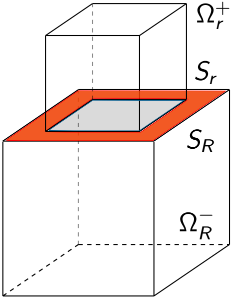
Energy density: $W(F) \sim \mathrm{dist}(F, \alpha SO(3))^2$

Elastic: $E_R^{el}(\theta) := \inf \left\{ \int_{\Omega_r^+} W(\nabla v)\, dx : \; v = x/\theta \text{ on } S_r \right\}$

Plastic: $E_R^{pl}(\theta) := \sigma \,\text{Area Gap} = \sigma R^2 (1 - \theta^2)$.

The energy functional: $E_R^{tot}(\theta) := E_R^{el}(\theta) + E_R^{pl}(\theta)$

$$E_R^{tot} := \min_\theta \left(E_R^{el}(\theta) + E_R^{pl}(\theta) \right)$$



Energy competition:

- $\theta = 1 \implies$ no dislocation energy
- $\theta = \alpha^{-1} \implies$ no elastic energy ($v := \alpha x$ admissible and $W(\alpha I) = 0$).

The asymptotic behaviour of E_R^{tot}

Let θ_R be the minimizer of E_R^{tot}, then as $R \to \infty$

$$E_R^{tot}(\theta_R) \to 0 \quad \text{and} \quad \theta_R \to \alpha^{-1} \implies \text{Linearization}$$

Set

$$\mathcal{E}^{el}(R) := \frac{\sigma^2}{\alpha^3 C^{el}} R\,, \qquad \mathcal{E}^{pl}(R) := \sigma R^2 \left(1 - \frac{1}{\alpha^2}\right) - 2\frac{\sigma^2}{\alpha^3 C^{el}} R\,.$$

Theorem (F., Palombaro, Ponsiglione (2015))

The following expansion of the total energy holds true (as $R \to +\infty$)

$$E_R^{el}(\theta_R) = \mathcal{E}^{el}(R) + O(R)\,, \qquad E_R^{pl}(\theta_R) = \mathcal{E}^{pl}(R) + O(R)$$

and in particular

$$E_R^{tot} = \mathcal{E}^{el}(R) + \mathcal{E}^{pl}(R) + o(R).$$

For large R dislocations are energetically more favorable, the spacing tends to $\delta = \frac{b}{\alpha - 1}$ and the far field stress is relieved.

G . Dal Maso, M. Negri and D. Percivale (2002).

Conclusions and perspectives

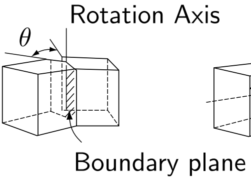
Conclusions:

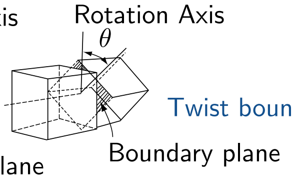
- A basic variational model describing the competition between the plastic energy spent at interfaces, and the corresponding release of bulk energy.
- The size of the overlayer is a free parameter $\implies$ free boundary problem, but only through the scalar parameter θ.

Perspectives:

- Grain boundaries, the misfit between the crystal lattices are described by rotations rather than dilations.
  W. T. Read and W. Shockley (1950) - J.P. Hirth and B. Carnahan (1992)
- Optimal geometry for the dislocation net (square vs hexagonal)
  M. Koslowski and M. Ortiz (2004)

Tilt boundary





Twist boundary