A Variational Model for Dislocations at Semi-Coherent Interfaces

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Semi-Coherent Interfaces

Polycrystal: two crystalline materials with different underlying lattice structures Λ^+ and Λ^-, $\Lambda^+ = \alpha\Lambda^-$, $\alpha > 1$. The lattice Λ^+ (overlayer) lies on top of Λ^- (underlayer) with flat interface.

Interface defects: Λ^+ and Λ^- have different densities, so near the interface many atoms have the "wrong" number of first neighbors (Fig 1a). Such atoms form *line singularities* corresponding to *edge dislocations*. Dislocations can be reduced by compressing Λ^+ near the interface (Fig 1c).

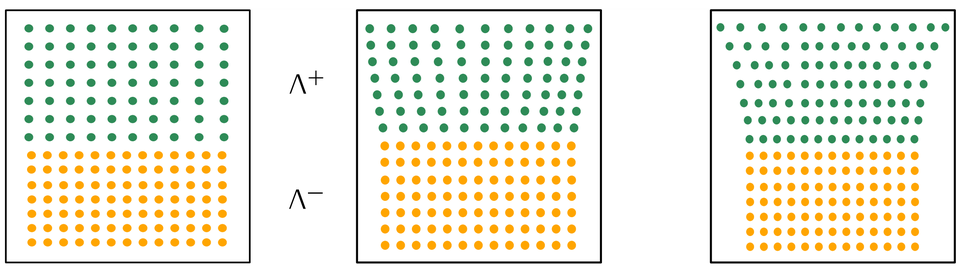

Fig 1. Cross section of the interface. 1a: stress-free. 1b: real minimizer. 1c: defect-free.

Energy scaling: competition between *Elastic Energy* and *Dislocation Energy* (Fig 1b):

- *Elastic Energy* scales like R^3 (volume of the body) for defect-free configurations.
- *Dislocation Energy* scales like R^2 (area of the interface).

Semi-coherent interfaces: $\Lambda^+ = \alpha\Lambda^-$ with misfit $\alpha \approx 1$. Example: heterostructured nanowires.

Large interfaces: semi-coherent interfaces show the following behavior for large R:

- Dislocations are energetically preferred over elastic strain .
- A Periodic Network of Edge Dislocations nucleates at the interface.

Semi-Discrete Model

Our analysis [1] builds on previous work done in [2].

Lattice structures: cubic lattice Λ^- with spacing $b > 0$, $\Lambda^+ := \alpha\Lambda^-$ with $\alpha := 1 + \frac{1}{n}$ fixed. Here b is independent of $R > 0$ diameter of the cross section.

Reference configuration:

- $\Omega_R := S_R \times (-hR, hR)$ cylinder with $h > 0$, $S_R := (-R/2, R/2)^2$ interface.
- $\Omega_R^+ := S_R \times (0, hR)$ overlayer with lattice Λ^+ not in equilibrium.
- $\Omega_R^- := S_R \times (-hR, 0)$ underlayer with lattice Λ^- already in equilibrium and assumed rigid.

Dislocations: we allow for nucleation of *edge dislocations* at the interface

- *Dislocation lines*: closed curves γ sitting on the grid $\mathcal{G} := \big((b\mathbb{Z} \times \mathbb{R}) \cup (\mathbb{R} \times b\mathbb{Z}) \cap S_R\big) \times \{0\}$.
- *Burgers vectors*: $\mathbf{b} \in \mathbb{R}^3$ belongs to the set of *slip directions* $b\mathbb{Z}\{e_1, e_2\}$.

The set of *admissible dislocations* is then

$$\mathcal{AD} := \{(\Gamma, \mathbf{B}) : \Gamma = \{\gamma_i\} \text{ finite family of curves } \gamma_i \subset \mathcal{G},\ \mathbf{B} = \{\mathbf{b}_i\} \text{ respective Burgers vectors}\} .$$

Deformations: maps $F : \Omega_R \to \mathbb{M}^{3\times 3}$. Dislocations are line defects of F. For $(\Gamma, \mathbf{B}) \in \mathcal{AD}$ admissible strains are

$$\mathcal{AS}(\Gamma, \mathbf{B}) := \left\{ F \in L^p_{\text{loc}}(\Omega_R; \mathbb{M}^{3\times 3}) : F = I \text{ in } \Omega_R^-,\ \operatorname{curl} F = -\textstyle\sum_i \mathbf{b}_i \otimes \dot{\gamma}_i \, d\mathcal{H}^1 \llcorner \gamma_i \right\} .$$

Energy: assume $W : \mathbb{M}^{3\times 3} \to [0, +\infty)$, continuous, frame indifferent and such that

$$W(F) \sim \operatorname{dist}^2(F; \alpha SO(3)) \wedge (|F|^p + 1) \quad \text{for some} \quad 1 < p < 2 .$$

- $E_R^{el} := \inf \left\{ \int_{\Omega_R^+} W(F(x))\, dx :\ F \in L^p_{\text{loc}}(\Omega_R)\,,\ F = I \text{ in } \Omega_R^-,\ \operatorname{curl} F = 0 \right\}$ (Elastic Energy)
- $E_R^{pl} := \min \left\{ \inf \left\{ \int_{\Omega_R^+} W(F(x))\, dx : F \in \mathcal{AS}(\Gamma, \mathbf{B}) \right\} : (\Gamma, \mathbf{B}) \in \mathcal{AD} \right\}$ (Dislocation Energy)

Scaling Properties of the Energies

Rigidity implies that

- $E_R^{el} > 0$ and $E_R^{pl} > 0$: matching the two phases always has a positive cost .
- $E_R^{el} = R^3\, E_1^{el}$: this shows that the elastic energy grows cubically $E_R^{el} \sim R^3$.

Characterizing the scaling of the dislocation energy E_R^{pl} is more delicate. We showed that:

Theorem 1. *There exists $0 < E^{pl} < +\infty$ such that*

$$E_R^{pl} = R^2\, E^{pl} + O(1) \quad \textit{where} \quad O(1) \to 0 \quad \textit{as} \quad R \to \infty . \qquad \square$$

Corollary 1. *Nucleation of Dislocations is energetically preferred for large interfaces.*
The optimal scaling for E_R^{pl} is obtained by introducing a Periodic Network of Edge Dislocations at the interface.

Periodic Network of Edge Dislocations

Construction: let $\delta := b/(\alpha - 1)$.

1. Divide S_R into $q \approx (R/\delta)^2$ squares Q_i with vertices in the lattice $S_R \cap \delta\mathbb{Z}^2$ and center x_i.
2. Above Q_i define pyramids: C_i^1 (height $\delta/2$), C_i^2 (height δ).
3. Deformation $v := x + u$ with displacement $u := 0$ in Ω_R^-, $u := (\alpha - 1)x$ in $\Omega_R^+ \setminus \cup_i C_i^2$, $u := (\alpha - 1)x_i$ in C_i^1 and linearly interpolate in $C_i^2 \setminus C_i^1$.

Dislocations: v has constant jump $(\alpha - 1)x_i$ across Q_i. Jumps induce dislocation lines $\gamma_{ij} := Q_i \cap Q_j$ with respective Burgers vectors $\mathbf{b}_{ij} := (\alpha - 1)(x_j - x_i)$, for adjacent Q_i and Q_j. If we define $\Gamma := \{\gamma_{ij}\}$ and $\mathbf{B} := \{\mathbf{b}_{ij}\}$ we have $(\Gamma, \mathbf{B}) \in \mathcal{AD}$ and $v \in \mathcal{AS}(\Gamma, \mathbf{B})$.

Proposition 1. $E_R^{pl} \le c\, R^2$ since $\int_{C_i^2} W(\nabla v(x))\, dx \le c\, \delta^3$.

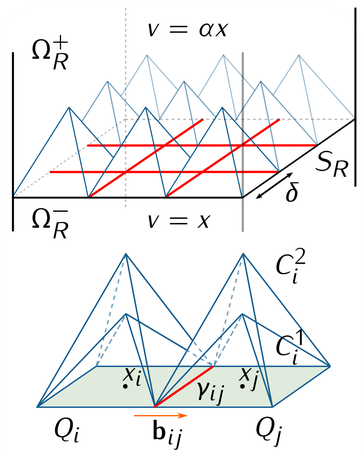

Fig 2. Double pyramids.

Some considerations

Drawback: if v is as above, $v(S_R)$ is union of squares of side δ separated by strips of width b (Fig 3). Some lines of atoms in $v(S_R)$ fall outside of S_R, suggesting this model is not appropriate to describe heterostructured materials.

Alternative: $\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+$ new reference configuration with $r := \theta R$ for $\theta \in (0, 1)$, enforcing $v(S_r) = S_R$ (Fig 1c). The above construction in $\Omega_{R,r}$ with $\delta = \frac{b}{\theta^{-1} - 1}$ yields $v(S_r) = S_R$.

Dislocation length: $L \approx \frac{1}{b} r^2(\theta^{-2} - 1) = \frac{1}{b} |S_R \setminus S_r|$ as $\theta \approx 1$.

Dislocation energy: $E_r^{pl} \approx \sigma_{\alpha,\theta}\, |S_R \setminus S_r|$ with $\sigma_{\alpha,\theta} := \frac{E^{pl}}{\theta^{-2} - 1}$
Dislocation energy is proportional to total dislocation length.

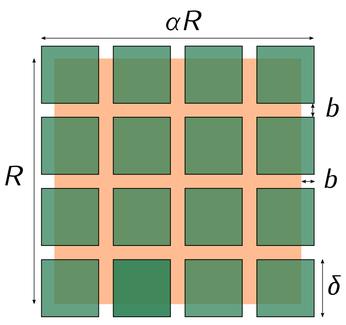

Fig 3. Interface mismatch.

Guess: for $r \to \infty$ and $\alpha \to 1^+$, E_r^{pl} is minimized by a periodic configuration of well separated dislocations. We then conjecture that $\lim_{\alpha \to 1^+} \sigma_{\alpha,\alpha^{-1}} =: \sigma$ for some $0 < \sigma < \infty$. We can interpret $b\sigma$ as the self energy of a single dislocation line per unit length.

Continuum Model

Reference Configuration: $\Omega_{R,r} := \Omega_R^- \cup S_r \cup \Omega_r^+$ with $R > 0$, $\theta \in [\alpha^{-1}, 1]$ and $r := \theta R$. Also fix $\sigma > 0$ (see above discussion).

Deformations: maps $v \in W^{1,2}(\Omega_r^+; \mathbb{R}^3)$ satisfying boundary condition $v(x) = \theta^{-1} x$ on S_r .

Energy: assume $W(F) \ge C\, \operatorname{dist}^2(F, \alpha SO(3))$ and $W(\alpha I) = 0$. Define energies:

- $E_R^{el}(\theta) := \inf \left\{ \int_{\Omega_r^+} W(\nabla v(x))\, dx :\ v \in W^{1,2}(\Omega_r^+; \mathbb{R}^3),\ v = \theta^{-1} x \text{ on } S_r \right\}$ (Elastic Energy)
- $E_R^{pl}(\theta) := \sigma R^2(1 - \theta^2)$ (proportional to mismatch area) (Dislocation Energy)
- $E_R^{tot}(\theta) := E_R^{el}(\theta) + E_R^{pl}(\theta)$ and $E_R^{tot} := \inf_{\theta \in [\alpha^{-1}, 1]} E_R^{tot}(\theta)$ (Total Energy)

Note 1. If $\theta = 1$ no dislocation energy is present. If $\theta = 1/\alpha$ no elastic energy is stored.

Note 2. E_R^{tot} *sub-quadratic*, that is $E_R^{tot} \le \sigma R^2(1 - \alpha^{-2})$.

Energy scaling: $E_R^{el}(1) \sim R^3$ by Rigidity.

Consider θ_R minimizing sequence, that is $E_R^{tot} = E_R^{tot}(\theta_R) + o(1)$ where $o(1) \to 0$ as $R \to +\infty$.

Corollary 2. Nucleation of Dislocations is preferred: $\theta_R < 1$ for large R.

Proposition 2. $E_1^{el}(\theta_R) \to 0$ and $\theta_R \to \alpha^{-1}$ as $R \to +\infty$.

Therefore we can linearize the Elastic Energy about αI (by Γ-convergence) and compute:

Theorem 2. (Taylor Expansion) There exists $C > 0$ (from linearized elasticity) such that

$$E_R^{tot} = E_C^{el}(R) + E_C^{pl}(R) + o(R)$$

where $o(R)/R \to 0$ as $R \to +\infty$ and

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

Bibliography

[1] S. Fanzon, M. Palombaro, and M. Ponsiglione. "A Variational Model for Dislocations at Semi-coherent Interfaces". In: *Journal of Nonlinear Science* 27.5 (2017), pp. 1435–1461.

[2] S. Müller and M. Palombaro. "Derivation of a rod theory for biphase materials with dislocaions at the interface". In: *Calc. Var. Partial Differential Equations* 48.3-4 (2013), pp. 315–335.