Linearised Polycrystals from a 2D System of Edge Dislocations

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in collaboration with

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Classical Elasticity: ideal crystals

Reference configuration: $\Omega \subset \mathbb{R}^3$ open bounded

Deformations: regular maps $v \colon \Omega \to \mathbb{R}^3$

Deformation strain: $\beta := \nabla v \colon \Omega \to \mathbb{M}^{3\times 3}$

Displacement: map $u \colon \Omega \to \mathbb{R}^3$ s.t. $v = x + u$

Nonlinear Elasticity: the energy associated to a deformation strain β is

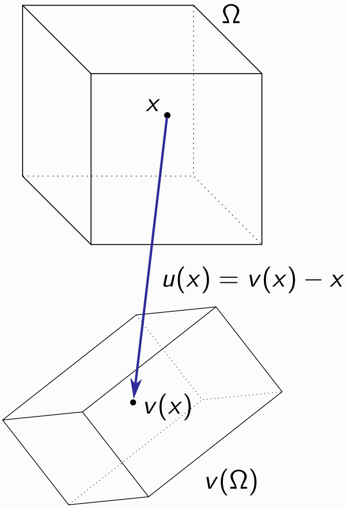
$$E(\beta) := \int_\Omega W(\beta)\, dx\,,$$

where $W(F) \sim \operatorname{dist}(F, SO(3))^2$ (so $W(I) = 0$).

Linear Elasticity: let $v = x + \varepsilon u$ with $\varepsilon \approx 0$. Then

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} \int_\Omega W(\beta)\, dx = \frac{1}{2} \int_\Omega \mathbb{C} \nabla^{\mathrm{sym}} u : \nabla^{\mathrm{sym}} u \, dx\,,$$

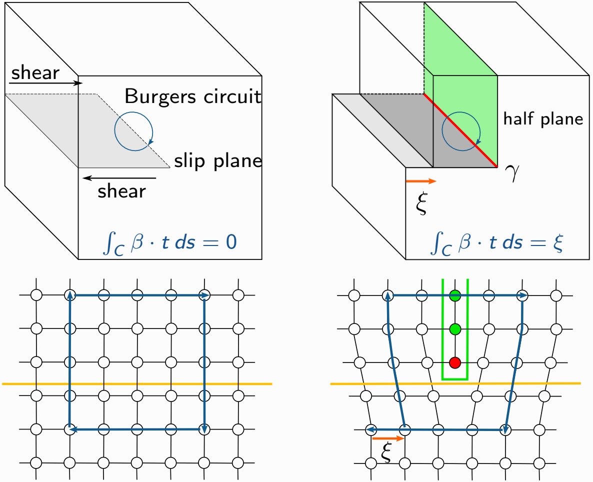
where $\mathbb{C} = \partial^2 W(I)$ and $\nabla^{\mathrm{sym}} u := (\nabla u + \nabla u^T)/2$.



Edge dislocations

Dislocations: topological defects in the otherwise periodic structure of a crystal.

Edge dislocation: pair (γ, ξ) of dislocation line and Burgers vector, with $\xi \perp \gamma$.



Adding dislocations: the semi-discrete model

Dislocation lines: Lipschitz curves $\gamma \subset \Omega$ such that $\Omega \setminus \gamma$ is not simply connected

Burgers vector: $\xi \in \mathcal{S}$ set of slip directions

Strain generating (γ, ξ): map $\beta \colon \Omega \to \mathbb{M}^{3\times 3}$ s.t.

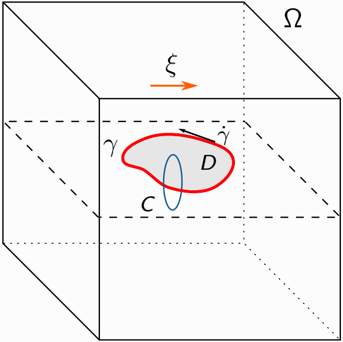
$$\operatorname{Curl} \beta = -\xi \otimes \dot\gamma \, \mathcal{H}^1 \llcorner \gamma \implies \int_C \beta \cdot t \, d\mathcal{H}^1 = \xi \, .$$

Geometric interpretation: if D encloses γ, there exists a deformation $v \in SBV(\Omega; \mathbb{R}^3)$ s.t.

$$Dv = \nabla v \, dx + \xi \otimes n \, \mathcal{H}^2 \llcorner D \, , \quad \beta = \nabla v \, .$$

In particular:

- $D =$ slip region,
- v has constant jump ξ across D,
- the absolutely continuous part of Dv is β.



Regularise the problem: Core Radius Approach

Let β generate (γ,ξ). Consider $\varepsilon > 0$ and

$$I_\varepsilon(\gamma) := \{x \in \mathbb{R}^3 : \ \mathrm{dist}(x,\gamma) < \varepsilon\}\,.$$

Then we have

$$|\beta(x)| \sim \frac{1}{\mathrm{dist}(x,\gamma)} \ \text{ in } \ I_\varepsilon(\gamma) \implies \beta \notin L^2(I_\varepsilon(\gamma)).$$

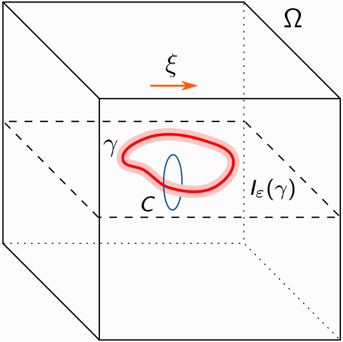
CRA: new ref. conf. $\Omega_\varepsilon(\gamma) := \Omega \setminus I_\varepsilon(\gamma)$.

New Strains: maps $\beta \in L^2(\Omega_\varepsilon(\gamma); \mathbb{M}^{3\times 3})$ s.t.

$$\mathrm{Curl}\,\beta \llcorner \Omega_\varepsilon(\gamma) = 0\,, \quad \int_C \beta \cdot t \, d\mathcal{H}^1 = \xi\,.$$

Elastic energy associated to β is

$$E_\varepsilon(\beta) := \int_{\Omega_\varepsilon(\gamma)} W(\beta)\, dx\,.$$



Γ-convergence

Let $\mathcal{X}$ be a metric space and $F_n \colon \mathcal{X} \to \mathbb{R} \cup \{\pm\infty\}$.

Definition (Γ-convergence)

We say that F_n Γ-converges to $F \colon \mathcal{X} \to \mathbb{R} \cup \{\pm\infty\}$ as $n \to \infty$ if:

- (Γ-liminf inequality) for every $x \in \mathcal{X}$ and every $\{x_n\}$ such that $x_n \to x$,
$$F(x) \leq \liminf_{n\to\infty} F_n(x_n)\,,$$
- (Γ-limsup inequality) for every $x \in \mathcal{X}$ there exists a recovery sequence $\{x_n\}$ such that $x_n \to x$ and
$$F(x) = \lim_{n\to\infty} F_n(x_n)\,.$$

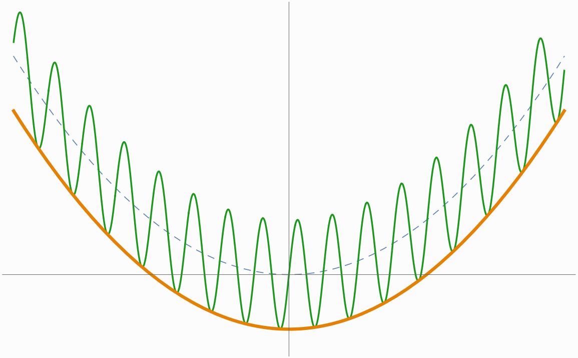
Theorem (Fundamental Theorem of Γ-convergence)

If $F_n \xrightarrow{\Gamma} F$ and $\{x_n\}$ are (almost) minimisers of F_n at each fixed n,

- *F admits minimum in $\mathcal{X}$ and $\inf_{\mathcal{X}} F_n \to \min_{\mathcal{X}} F$*
- *if $x_n \to x$ then $F(x) = \min_{\mathcal{X}} F$.*

Γ-convergence: basic example

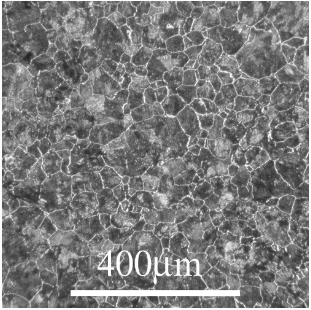
Let $\mathcal{X} = \mathbb{R}$ and define $F_n(x) := x^2 + \cos(nx)$.



We have that $F_n \xrightarrow{\Gamma} F := x^2 - 1$ as $n \to \infty$.

Motivation: polycrystals

Polycrystal: formed by many grains, having the **same** lattice structure, mutually rotated $\Longrightarrow$ interface misfit at **grain boundaries**.



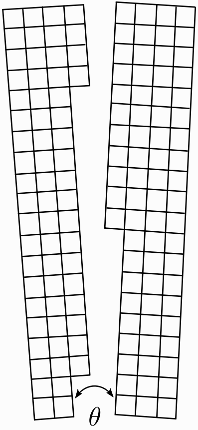
Goal: to obtain polycrystalline structures as minimisers of some energy functional.

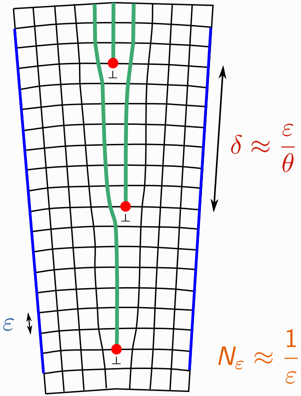
Fanzon, Palombaro, Ponsiglione. *Derivation of Linearized Polycrystals from a Two-Dimensional System of Edge Dislocations.* SIMA (2019)

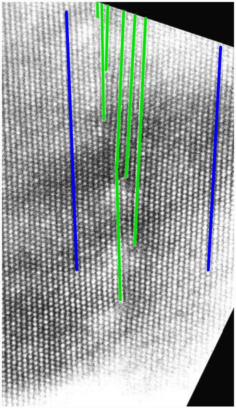
Structure of Tilt Grain Boundaries

Tilt boundary: small angle rotation θ between grains $\implies$ **edge dislocations**.

Boundary structure: periodic array of edge dislocations with spacing $\boldsymbol{\delta = \varepsilon/\theta}$.







Porter, Easterling. CRC Press (2009) - Gottstein. Springer (2013)

Plan of the paper

Setting: consider a 2D system of N_ε edge dislocations, where $\varepsilon > 0$ is the lattice spacing and

$$N_\varepsilon \to +\infty \quad \text{as} \quad \varepsilon \to 0\,.$$

Plan: let $\mathcal{F}_\varepsilon$ be the energy of such system.

- We compute $\mathcal{F}$, the Γ-limit of $\mathcal{F}_\varepsilon$ as $\varepsilon \to 0$,
- we show that under suitable boundary conditions $\mathcal{F}$ is minimised by polycrystals.

Linearised polycrystals: our energy regime will imply

$$N_\varepsilon \ll \frac{1}{\varepsilon}$$

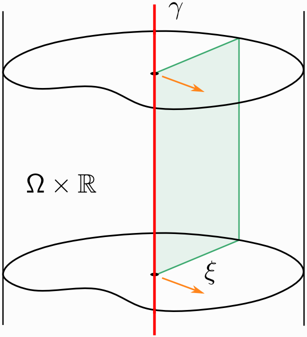
$\implies$ we have less dislocations than tilt grain boundaries. However we still obtain polycrystalline minimisers, but with grains rotated by an infinitesimal angle $\theta \approx 0$.

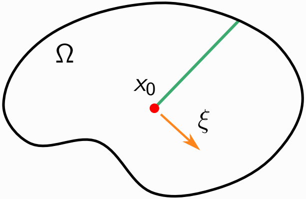
Setting: linear planar elasticity

Reference configuration: $\Omega \subset \mathbb{R}^2$ open bounded.

Dislocation lines: points $x_0 \in \Omega$ separated by 2ε.

Burgers vectors: finite set $\mathcal{S} := \{b_1, \ldots, b_s\} \subset \mathbb{R}^2$.





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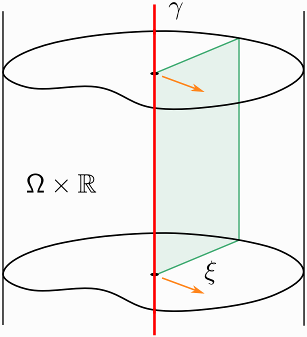
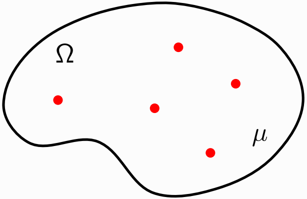
Admissible dislocations: finite sums of Dirac masses

$$\mu := \sum_{i=1}^{N} \xi_i \, \delta_{x_i} \,, \quad \xi_i \in \mathcal{S} \,.$$





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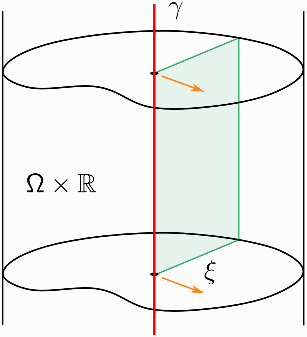

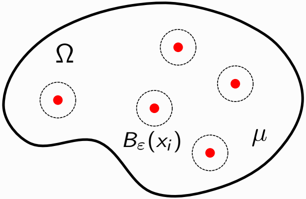

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Strains: inducing μ are maps $\beta \colon \Omega_\varepsilon(\mu) \to \mathbb{M}^{2\times 2}$ s.t. $\beta = 0$ in $\cup B_\varepsilon(x_i)$ and

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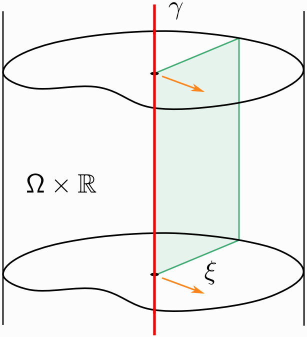

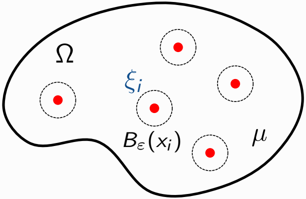

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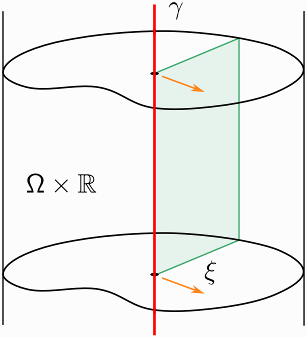

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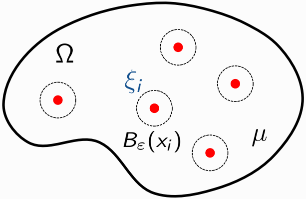
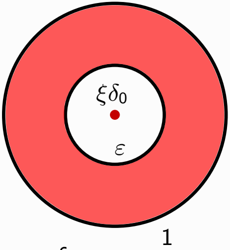
Linear Energy: $\mathbb{C}F : F \sim |F^{\mathrm{sym}}|^2$, then

$$E_\varepsilon(\mu, \beta) := \int_\Omega \mathbb{C}\beta : \beta \, dx = \int_\Omega \mathbb{C}\beta^{\mathrm{sym}} : \beta^{\mathrm{sym}} \, dx \,.$$



Self-energy of a single dislocation core

Let β generate $\xi\,\delta_0$, that is "$\mathrm{Curl}\,\beta = \xi\,\delta_0$"



$$\int_{B_1\setminus B_\varepsilon} |\beta|^2\,dx \geq \int_\varepsilon^1 \int_{\partial B_\rho} |\beta\cdot t|^2\,ds\,d\rho \geq \text{(Jensen)}$$

$$\geq \frac{1}{2\pi}\int_\varepsilon^1 \frac{1}{\rho}\left|\int_{\partial B_\rho} \beta\cdot t\,ds\right|^2 d\rho = \frac{|\xi|^2}{2\pi}|\log\varepsilon|\,.$$

The reverse inequality can be obtained by computing the energy of

$$\beta(x) := \frac{1}{2\pi}\,\xi\otimes J\frac{x}{|x|^2}\,, \quad J := \text{clock-wise rotation of } \frac{\pi}{2}\,.$$

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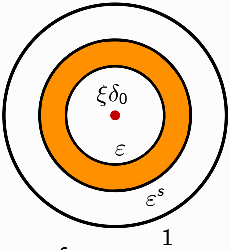

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Remark: let $s \in (0,1)$, then

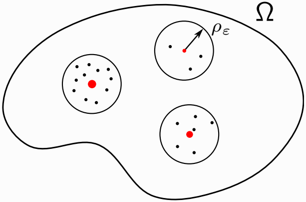
$$\int_{B_{\varepsilon^s} \setminus B_\varepsilon} |\beta|^2\,dx \geq (1-s)\frac{|\xi|^2}{2\pi} |\log \varepsilon|\,.$$

Self-energy: is of order $|\log \varepsilon|$ and concentrated in a small region around B_ε.

The Hard Core assumption

HC Radius: fixed scale $\rho_\varepsilon \gg \varepsilon$ with $\rho_\varepsilon \to 0$.

Clusters of dislocations at scale ρ_ε are identified with a single **multiple dislocation**.



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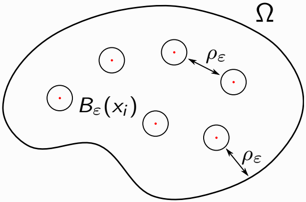
Admissible dislocations: finite sums of Dirac masses

$$\mu := \sum_{i=1}^{N} \xi_i \, \delta_{x_i} \,, \quad \xi_i \in \mathbb{S} \,,$$

with $\mathbb{S} := \mathrm{Span}_{\mathbb{Z}} \, \mathcal{S}$ set of multiple Burgers vectors, and

$$|x_i - x_j| > 2\rho_\varepsilon \,, \quad \mathrm{dist}(x_k, \partial\Omega) > \rho_\varepsilon \,.$$



Note: dislocations separation is a technical assumption for energy estimates.

Hypothesis on HC Radius: as $\varepsilon \to 0$

- $\rho_\varepsilon / \varepsilon^s \to \infty, \ \forall \, s \in (0,1)$, (HC region contains almost all the self-energy)
- $N_\varepsilon \rho_\varepsilon^2 \to 0$. (Measure of HC region vanishes)

Energy regimes

Energy scaling: each dislocation accounts for $|\log\varepsilon| \implies$ relevant scaling is

$$E_\varepsilon \approx N_\varepsilon |\log\varepsilon| \,.$$

Rescaled energy functionals:

$$\mathcal{F}_\varepsilon(\mu,\beta) := \frac{1}{N_\varepsilon|\log\varepsilon|}\int_{\Omega_\varepsilon(\mu)} \mathbb{C}\beta^{\rm sym} : \beta^{\rm sym}\, dx \,.$$

Energy regimes: the behaviour of N_ε determines three different regimes:

- $N_\varepsilon \ll |\log\varepsilon| \rightsquigarrow$ Dilute dislocations
- $N_\varepsilon \approx |\log\varepsilon| \rightsquigarrow$ Critical regime

  Garroni, Leoni, Ponsiglione. *Gradient theory for plasticity via homogenization of discrete dislocations.* J. Eur. Math. Soc. (JEMS) (2010)

- $N_\varepsilon \gg |\log\varepsilon| \rightsquigarrow$ Super-critical regime

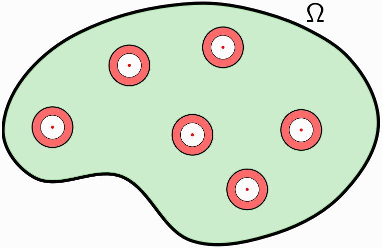
  Fanzon, Palombaro, Ponsiglione. *Derivation of Linearized Polycrystals from a Two-Dimensional System of Edge Dislocations.* SIMA (2019)

Behaviour of $\mathcal{F}_\varepsilon$ as $\varepsilon \to 0$ (Heuristic)

Let (μ, β) with $\mu = \sum_{i=1}^{N_\varepsilon} \xi_i \, \delta_{x_i}$ be such that "Curl $\beta = \mu$".

Energy decomposition: let $\mathrm{HC}_\varepsilon(\mu) := \cup_{\mathrm{i}=1}^{\mathrm{N}_\varepsilon} \mathrm{B}_{\rho_\varepsilon}(\mathrm{x_i})$ be the HC region

$$E_\varepsilon(\mu, \beta) = \int_{\Omega \setminus \mathrm{HC}_\varepsilon(\mu)} \mathbb{C}\beta : \beta \, dx + \int_{\mathrm{HC}_\varepsilon(\mu)} \mathbb{C}\beta : \beta \, dx = E_\varepsilon^{\mathrm{interaction}} + E_\varepsilon^{\mathrm{self}} \, .$$



Idea: rescaling by $N_\varepsilon |\log \varepsilon|$, we have $E_\varepsilon^{\mathrm{interaction}} \to E^{\mathrm{elastic}}$ and $E_\varepsilon^{\mathrm{self}} \to E^{\mathrm{plastic}}$.

Γ-convergence result for $N_\varepsilon \gg |\log \varepsilon|$

Theorem (Fanzon, Palombaro, Ponsiglione '19)

Compactness: *consider* $(\mu_\varepsilon, \beta_\varepsilon)$ *s.t.* "$\operatorname{Curl} \beta_\varepsilon = \mu_\varepsilon$" *and* $\mathcal{F}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon) \leq C \implies$

- $\dfrac{\beta_\varepsilon^{\mathrm{sym}}}{\sqrt{N_\varepsilon |\log \varepsilon|}} \rightharpoonup S\,, \quad \dfrac{\beta_\varepsilon^{\mathrm{skew}}}{N_\varepsilon} \rightharpoonup A$ *in* $L^2(\Omega; \mathbb{M}^{2\times 2})$,
- $\dfrac{\mu_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu$ *in* $\mathcal{M}(\Omega; \mathbb{R}^2)$,
- $\operatorname{Curl} A = \mu$ *and* $\mu \in H^{-1}(\Omega; \mathbb{R}^2)$ $(\implies A \in BV(\Omega; \mathbb{M}^{2\times 2}_{\mathrm{skew}}))$.

Γ-convergence: *the functionals* $\mathcal{F}_\varepsilon$ Γ*-converge to*

$$\mathcal{F}(\mu, S, A) := \int_\Omega \mathbb{C} S : S \, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|\,, \quad \text{with } \operatorname{Curl} A = \mu\,.$$

Remark:

- S and A live on two different scales with $S \ll A \implies$ terms in $\mathcal{F}$ decoupled.
- In the critical regime $N_\varepsilon \approx |\log \varepsilon|$ we have $S \approx A$ and $\operatorname{Curl}(S + A) = \mu$.

The relaxation formula for φ

Self-energy for a single dislocation core $\xi\delta_0$ is

$$\psi(\xi) := \lim_{\varepsilon \to 0} \min_{\beta} \left\{ \frac{1}{|\log \varepsilon|} \int_{B_1 \setminus B_\varepsilon} \mathbb{C}\beta : \beta \, dx : \text{ ``}\operatorname{Curl} \beta = \xi\delta_0\text{''} \right\} .$$

Plastic density: the map $\varphi \colon \mathbb{R}^2 \to [0, \infty)$ defined as the relaxation of ψ

$$\varphi(\xi) := \min \left\{ \sum_{i=1}^{M} \lambda_i \psi(\xi_i) : \, \xi = \sum_{i=1}^{M} \lambda_i \xi_i, \, M \in \mathbb{N}, \, \lambda_i \geq 0, \, \xi_i \in \mathbb{S} \right\} .$$

Note: since the energy is quadratic, in the Γ-limit we have φ instead of ψ.

Properties: φ is convex and positively 1-homogeneous. Moreover $\exists \; c > 0$ s.t.

$$c^{-1} |\xi| \leq \varphi(\xi) \leq c \, |\xi| \, , \quad \forall \, \xi \in \mathbb{R}^2 \, .$$

Ideas for compactness: measures

Let $(\mu_\varepsilon, \beta_\varepsilon)$ with $\mu_\varepsilon = \sum_{i=1}^{M_\varepsilon} \xi_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$ and "$\mathrm{Curl}\,\beta_\varepsilon = \mu_\varepsilon$". Assume that

$$\sup_\varepsilon \mathcal{F}_\varepsilon(\mu_\varepsilon, \beta_\varepsilon) \leq C\,.$$

We show that

$$\frac{|\mu_\varepsilon|(\Omega)}{N_\varepsilon} = \frac{1}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon} |\xi_{\varepsilon,i}| \leq C \implies \frac{\mu_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu\,. \tag{1}$$

$$C \geq \frac{1}{N_\varepsilon |\log\varepsilon|}\int_\Omega \mathbb{C}\beta_\varepsilon : \beta_\varepsilon\,dx \geq \frac{1}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon} \frac{1}{|\log\varepsilon|}\int_{B_{\rho_\varepsilon}(x_{\varepsilon,i})} \mathbb{C}\beta_\varepsilon : \beta_\varepsilon\,dx$$

$$(\rho_\varepsilon \gg \varepsilon) \gtrsim \frac{1}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon} \psi(\xi_{\varepsilon,i}) \geq \frac{1}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon} \varphi(\xi_{\varepsilon,i}) = \frac{1}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon} |\xi_{\varepsilon,i}|\,\varphi\left(\frac{\xi_{\varepsilon,i}}{|\xi_{\varepsilon,i}|}\right)$$

$$\left(c := \min_{|\xi|=1}\varphi(\xi) > 0\right) \geq \frac{c}{N_\varepsilon}\sum_{i=1}^{M_\varepsilon} |\xi_{\varepsilon,i}| = \frac{c}{N_\varepsilon}|\mu_\varepsilon|(\Omega) \implies (1)$$

Ideas for compactness: strains

Symmetric Part: recalling that $\mathbb{C}F : F \geq C|F^{\mathrm{sym}}|^2$, we have

$$N_\varepsilon |\log \varepsilon| \geq C \int_\Omega \mathbb{C}\beta_\varepsilon : \beta_\varepsilon \, dx \geq C \int_\Omega |\beta_\varepsilon^{\mathrm{sym}}|^2 \, dx \implies \frac{\beta_\varepsilon^{\mathrm{sym}}}{\sqrt{N_\varepsilon |\log \varepsilon|}} \rightharpoonup S \, .$$

Skew Part: we use a Generalised Korn inequality: there exists $C > 0$ s.t. for every $\beta \in L^1(\Omega; \mathbb{M}^{2\times 2})$ with $\mathrm{Curl}\, \beta \in \mathcal{M}(\Omega; \mathbb{R}^2)$,

$$\int_\Omega |\beta^{\mathrm{skew}}|^2 \, dx \leq C \left(\int_\Omega |\beta^{\mathrm{sym}}|^2 \, dx + |\,\mathrm{Curl}\, \beta|(\Omega)^2 \right) . \tag{2}$$

Since "$\mathrm{Curl}\, \beta_\varepsilon = \mu_\varepsilon$", by (2) and assumption $N_\varepsilon \gg |\log \varepsilon|$ we get

$$\begin{aligned} \int_\Omega |\beta_\varepsilon^{\mathrm{skew}}|^2 \, dx &\leq C \left(\int_\Omega |\beta_\varepsilon^{\mathrm{sym}}|^2 \, dx + |\mu_\varepsilon|(\Omega)^2 \right) \\ &\leq C \left(N_\varepsilon |\log \varepsilon| + N_\varepsilon^2 \right) \leq C N_\varepsilon^2 \implies \frac{\beta_\varepsilon^{\mathrm{skew}}}{N_\varepsilon} \rightharpoonup A. \end{aligned}$$

Garroni, Leoni, Ponsiglione. J. Eur. Math. Soc. (JEMS) (2010)

Ideas for Γ-liminf

Assume that $(\mu_\varepsilon, \beta_\varepsilon)$ is such that $\mu_\varepsilon = \sum_{i=1}^{M_\varepsilon} \xi_{\varepsilon,i}\delta_{x_{\varepsilon,i}}$, "Curl $\beta_\varepsilon = \mu_\varepsilon$" and

$$\frac{\beta_\varepsilon^{\rm sym}}{\sqrt{N_\varepsilon |\log \varepsilon|}} \rightharpoonup S\,, \quad \frac{\beta_\varepsilon^{\rm skew}}{N_\varepsilon} \rightharpoonup A\,, \quad \frac{\mu_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu\,, \quad \text{with } \operatorname{Curl} A = \mu\,.$$

We have to show

$$\liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon |\log\varepsilon|} \int_\Omega \mathbb{C}\beta_\varepsilon : \beta_\varepsilon \, dx \geq \int_\Omega \mathbb{C}S : S\, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|\,.$$

Idea: split the energy $E_\varepsilon(\mu_\varepsilon, \beta_\varepsilon) = E_\varepsilon^{\rm interaction} + E_\varepsilon^{self}$ and use lower semicontinuity:

$$\liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon |\log\varepsilon|} \int_{\Omega\setminus HC_\varepsilon} \mathbb{C}\beta_\varepsilon : \beta_\varepsilon \, dx \geq \int_\Omega \mathbb{C}S : S\, dx \quad (N_\varepsilon \rho_\varepsilon^2 \to 0 \implies |HC_\varepsilon| \to 0)$$

$$\liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon |\log\varepsilon|} \int_{HC_\varepsilon} \mathbb{C}\beta_\varepsilon : \beta_\varepsilon \, dx = \liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon} \sum_{i=1}^{M_\varepsilon} \frac{1}{|\log\varepsilon|} \int_{B_{\rho_\varepsilon}(x_{\varepsilon,i})} \mathbb{C}\beta_\varepsilon : \beta_\varepsilon \, dx$$

$$\gtrsim \liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon} \sum_{i=1}^{M_\varepsilon} \varphi(\xi_{\varepsilon,i}) = \liminf_{\varepsilon\to 0} \frac{1}{N_\varepsilon} \int_\Omega \varphi\left(\frac{d\mu_\varepsilon}{d|\mu_\varepsilon|}\right) d|\mu_\varepsilon| \geq \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|$$

by Reshetnyak's lower semicontinuity Theorem, since φ is 1-homogeneous.

Ideas for Γ-limsup

Consider (μ, S, A) with S symmetric, A skew and $\operatorname{Curl} A = \mu$. We have to construct a recovery sequence $(\mu_\varepsilon, \beta_\varepsilon)$ with "$\operatorname{Curl} \beta_\varepsilon = \mu_\varepsilon$" s.t.

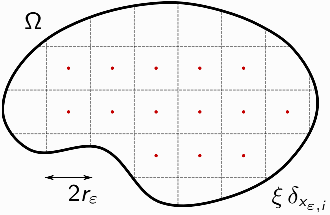
$$\frac{\beta_\varepsilon^{\mathrm{sym}}}{\sqrt{N_\varepsilon |\log \varepsilon|}} \rightharpoonup S \,, \quad \frac{\beta_\varepsilon^{\mathrm{skew}}}{N_\varepsilon} \rightharpoonup A \,, \quad \frac{\mu_\varepsilon}{N_\varepsilon} \overset{*}{\rightharpoonup} \mu \,, \tag{3}$$

$$\lim_{\varepsilon \to 0} \frac{1}{N_\varepsilon |\log \varepsilon|} \int_\Omega \mathbb{C}\beta_\varepsilon : \beta_\varepsilon \, dx = \int_\Omega \mathbb{C}S : S \, dx + \int_\Omega \varphi \left(\frac{d\mu}{d|\mu|} \right) d|\mu| \,. \tag{4}$$

For simplicity assume $\mu = \xi \, dx$ with $\varphi(\xi) = \psi(\xi)$. The general is more technical.

Recovery measures:

- divide Ω in $\approx N_\varepsilon$ squares of side $2r_\varepsilon = C/\sqrt{N_\varepsilon}$
- the recovery sequence is $\mu_\varepsilon = \sum_{i=1}^{M_\varepsilon} \xi \delta_{\varepsilon,i}$.



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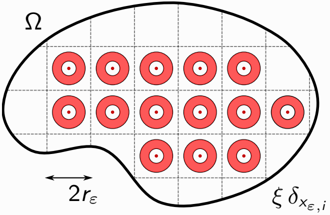


Recovery strains: let K_ε be the solution to the cell-problem about each $x_{\varepsilon,i}$. Then $K_\varepsilon / \sqrt{N_\varepsilon |\log \varepsilon|} \rightharpoonup 0$ and

$$\beta_\varepsilon = \sqrt{N_\varepsilon |\log \varepsilon|} S + N_\varepsilon A + K_\varepsilon + O(\sqrt{N_\varepsilon |\log \varepsilon|})$$

satisfies (3), (4) and "$\operatorname{Curl} \beta_\varepsilon = \mu_\varepsilon$".

Adding boundary conditions

Dirichlet type BC: at level $\varepsilon > 0$ fix a boundary condition $g_\varepsilon \colon \Omega \to \mathbb{M}^{2\times 2}$ s.t.

$$\frac{g_\varepsilon^{\mathrm{sym}}}{\sqrt{N_\varepsilon |\log \varepsilon|}} \rightharpoonup g_S \,, \qquad \frac{g_\varepsilon^{\mathrm{skew}}}{N_\varepsilon} \rightharpoonup g_A \,.$$

Dislocations and strains: (μ, β) such that " Curl $\beta = \mu$" and

$$\mu(\Omega) = \int_{\partial\Omega} g_\varepsilon \cdot t \, ds \,, \qquad \beta \cdot t = g_\varepsilon \cdot t \quad \text{on} \quad \partial\Omega \,.$$

Theorem (Fanzon, Palombaro, Ponsiglione '19)

The energy functionals $\mathcal{F}_\varepsilon$ are equi-coercive and they Γ-converge to

$$\mathcal{F}_{\mathrm{BC}}(\mu, S, A) := \int_\Omega \mathbb{C} S : S \, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu| + \int_{\partial\Omega} \varphi((g_A - A)\cdot t)\, ds \,,$$

with Curl $A = \mu$ *and* $\mu \in \mathcal{M}(\Omega; \mathbb{R}^2) \cap H^{-1}(\Omega; \mathbb{R}^2)$.

Remark: $\beta^{\mathrm{sym}} \ll \beta^{\mathrm{skew}} \implies$ BC pass to the limit only for A.

Minimising $\mathcal{F}_{\rm BC}$ with piecewise constant BC

Remark: there are no BC on $S \implies$ we can neglect elastic energy.

Piecewise constant BC: Fix a piecewise constant BC

$$g_A := \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix}, \quad a := \sum_{k=1}^{M} m_k \, \chi_{U_k} \,,$$

with $m_k < m_{k+1}$ and $\{U_k\}_{k=1}^M$ Caccioppoli partition of Ω.

Problem

Minimise

$$\mathcal{F}_{\rm BC}(\operatorname{Curl} A, 0, A) = \int_\Omega \varphi\left(\frac{d \operatorname{Curl} A}{d|\operatorname{Curl} A|}\right) \, d|\operatorname{Curl} A| + \int_{\partial\Omega} \varphi((g_A - A)\cdot t)\, ds\,,$$

with $\operatorname{Curl} A \in \mathcal{M}(\Omega;\mathbb{R}^2) \cap H^{-1}(\Omega;\mathbb{R}^2)$.

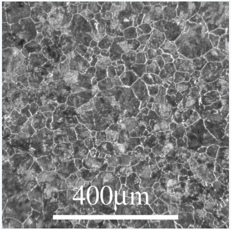
Polycrystals as energy minimisers

Theorem (Fanzon, Palombaro, Ponsiglione '19)

Given a piecewise constant boundary condition g_A, there exists a piecewise constant minimiser of $\mathcal{F}_{\mathrm{BC}}(\operatorname{Curl} A, 0, A)$

$$A = \sum_{k=1}^{M} A_k \chi_{E_k} \,,$$

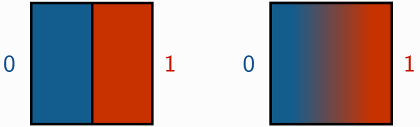
with $A_k \in \mathbb{M}^{2\times 2}_{\mathrm{skew}}$ and $\{E_k\}_{k=1}^{M}$ Caccioppoli partition of Ω. We interpret A as a linearised polycrystal.



Proof Strategy: We are minimising an anisotropic total variation functional. By Coarea formula we select the levels with minimal perimeter, definying the Caccioppoli partition.

Open Question: Are all minimisers piecewise constant? Uniqueness?

Essential: that the boundary condition is piecewise affine on the whole $\partial\Omega$.



Conclusions and Perspectives

Conclusions:

- A variational model for linearised polycrystals with infinitesimal rotations between the grains, deduced by Γ-convergence.
- Networks of dislocations are obtained as the result of energy minimisation, under suitable boundary conditions.

Open Questions:

- Uniqueness of piecewise constant minimisers?
- Dynamics for linearised polycrystals?
  Taylor. Bull. Amer. Math. Soc. (1978).
  Chambolle, Morini, Ponsiglione. Comm. Pure Appl. Math (2017).
- Γ-convergence analysis starting from a non-linear energy?
  Namely, considering small deformations $v = x + \varepsilon u$. Now the Burgers vectors are $\varepsilon \xi$ and the equivalent rescaling is $\varepsilon^2 N_\varepsilon |\log \varepsilon|$.
  Müller, Scardia, Zeppieri. Indiana University Mathematics Journal (2014).

Thank You!