Linearised Polycrystals from a 2D System of Edge Dislocations

Silvio Fanzon

in collaboration with

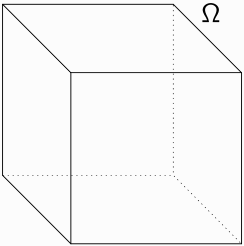
M. Palombaro and M. Ponsiglione

Graz, 31st January 2018

UNIVERSITY OF SUSSEX

Classical Elasticity: ideal crystals

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



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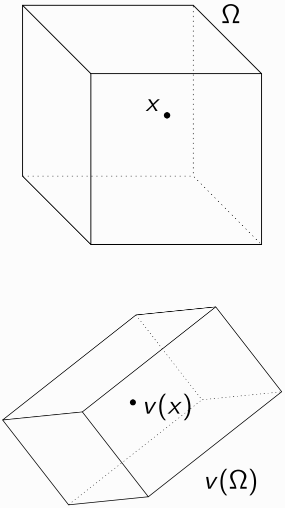

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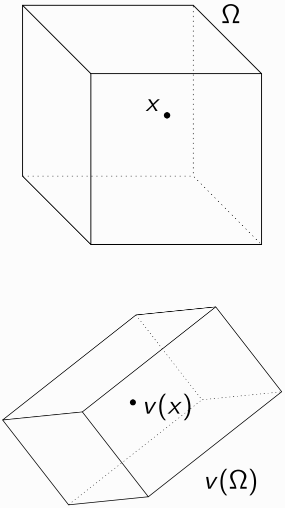

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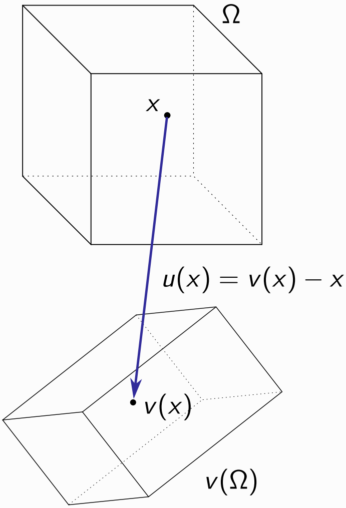

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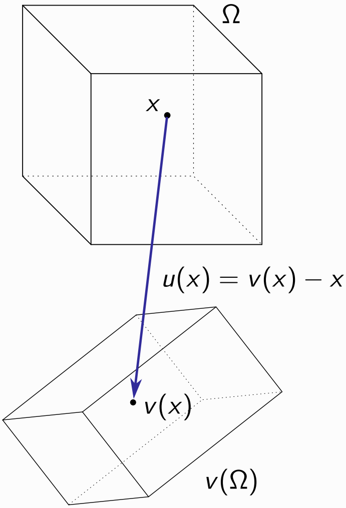
Nonlinear Elasticity: the energy associated to a deformation strain β is

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

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



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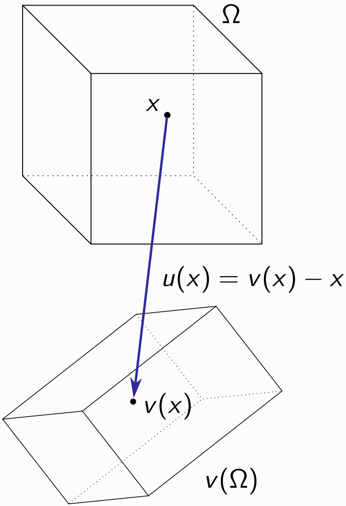
Linear Elasticity: let $v = x + \varepsilon u$ with $\varepsilon \approx 0$. Then

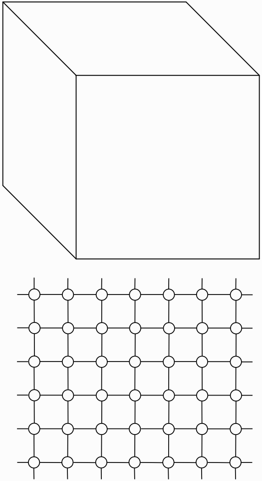
$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} \int_\Omega W(\beta)\, dx = \frac{1}{2} \int_\Omega \mathbb{C} \nabla^{\mathrm{sym}} u : \nabla^{\mathrm{sym}} u \, dx \,,$$

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.



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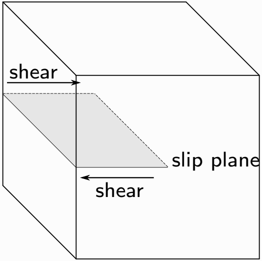

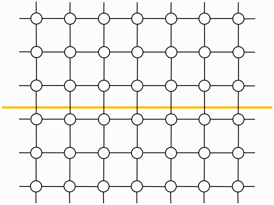

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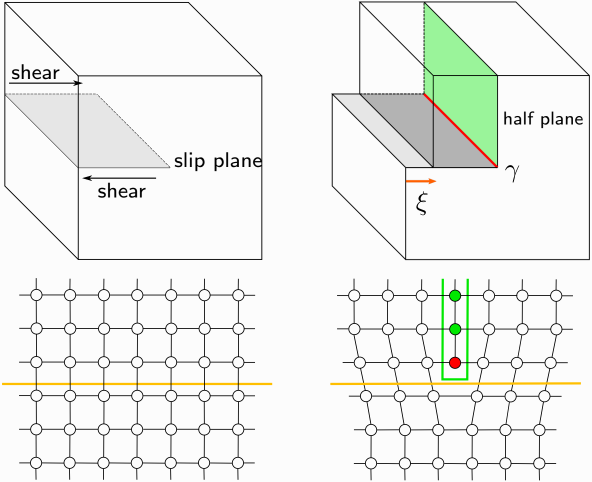

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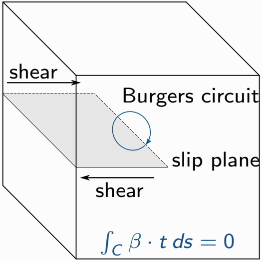

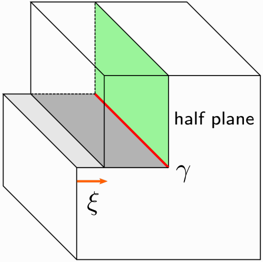

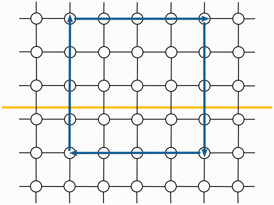

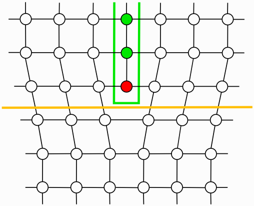

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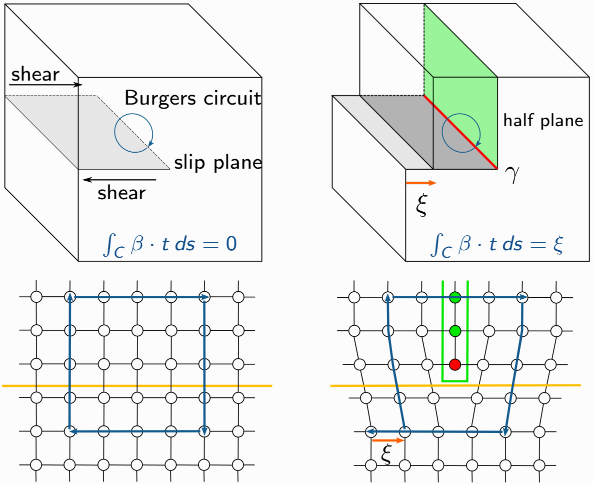
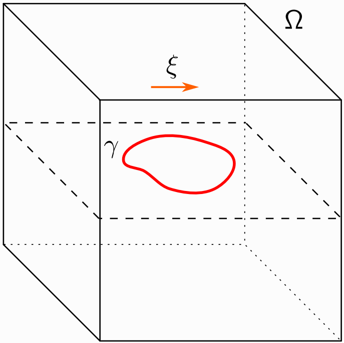


Adding dislocations: the semi-discrete model

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



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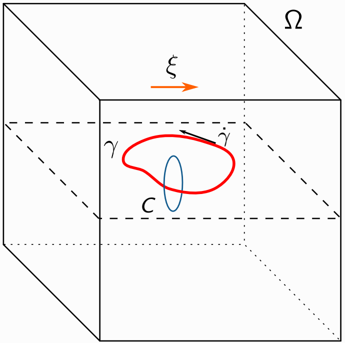

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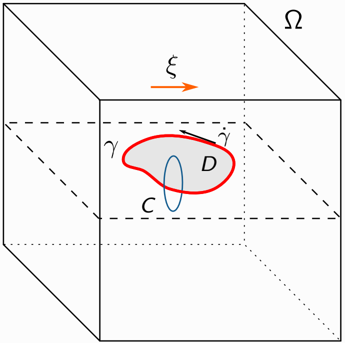
Geometric interpretation: if D encloses γ, there exists a deformation $v \in SBV(\Omega; \mathbb{R}^3)$ s.t.

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

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

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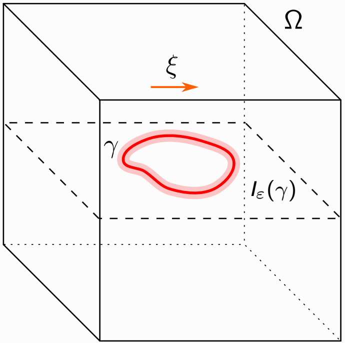

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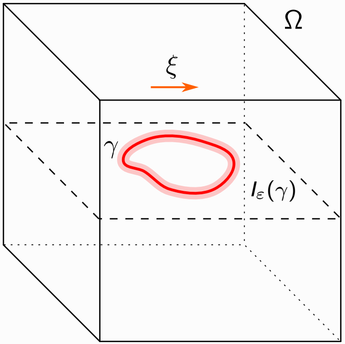

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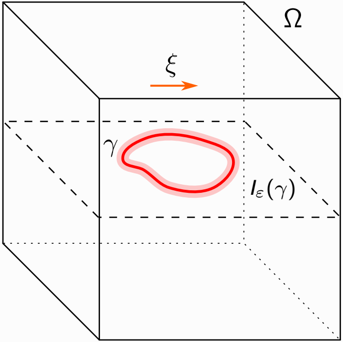

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New Strains: maps $\beta \in L^2(\Omega_\varepsilon(\gamma); \mathbb{M}^{3\times3})$ s.t.

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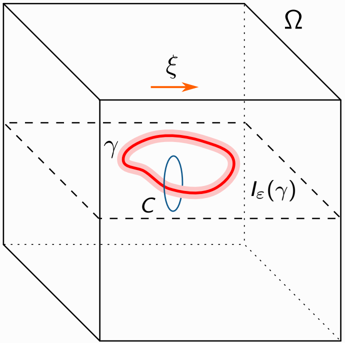

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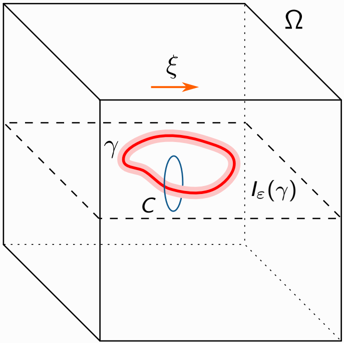

Elastic energy associated to β is

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

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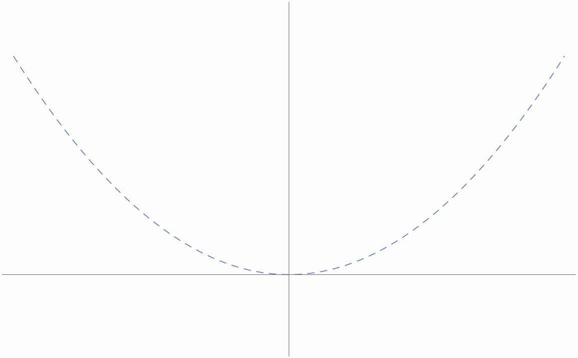
- *if $x_n \to x$ then $F(x) = \min_{\mathcal{X}} F$.*

Γ-convergence: basic example

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



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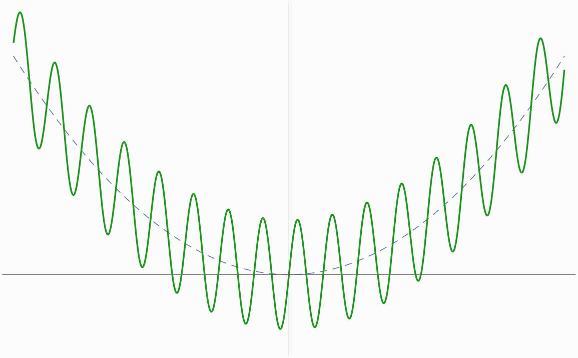

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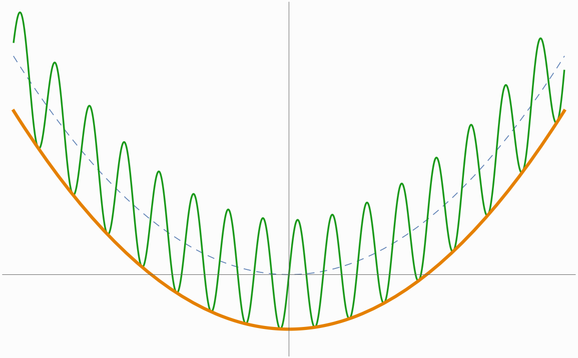
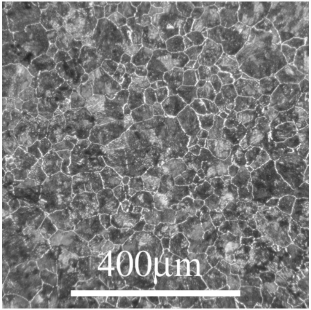


We have that $F_n \xrightarrow{\Gamma} F := x^2 - 1$ as $n \to \infty$.

Motivation: polycrystals

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



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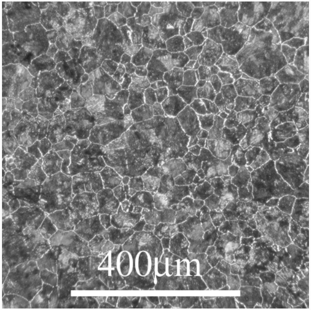


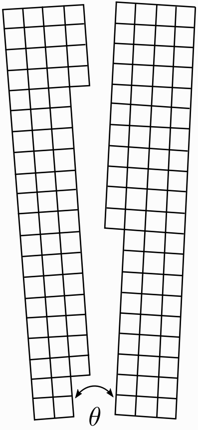
Goal: to obtain polycrystalline structures as minimisers of some energy functional.

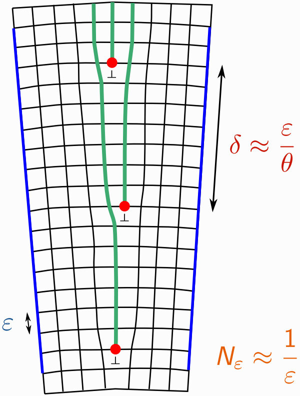
F., Palombaro, Ponsiglione. *Linearised Polycrystals from a 2D System of Edge Dislocations.* Preprint (2017)

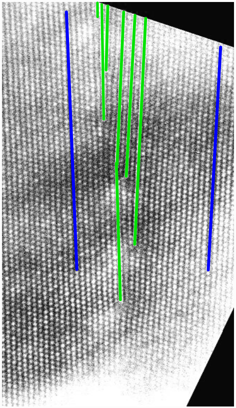
Structure of Tilt Grain Boundaries

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

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







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

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Linearised polycrystals: our energy regime will imply

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

$\Longrightarrow$ 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

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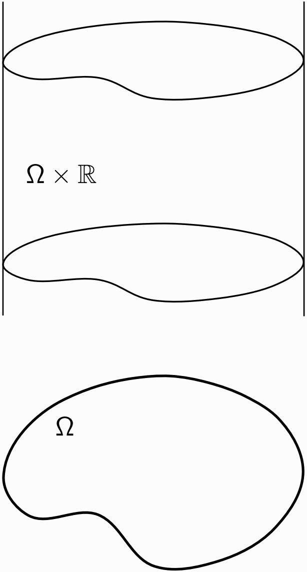

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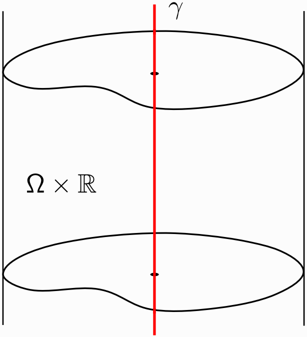

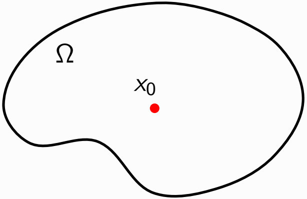

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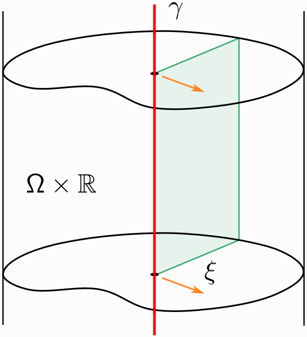

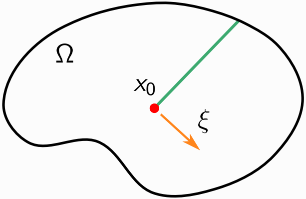

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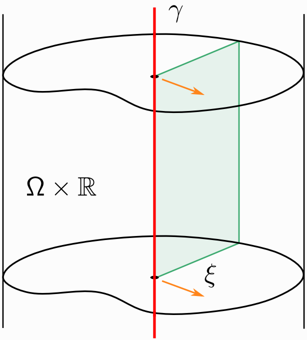

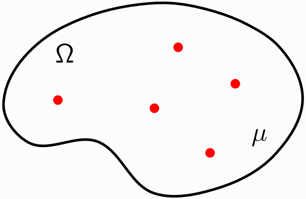

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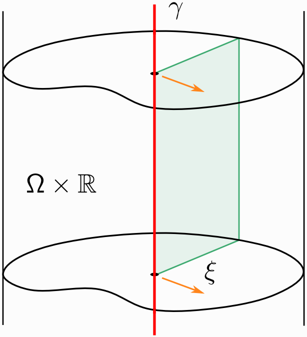

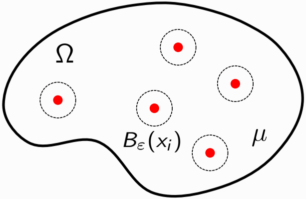

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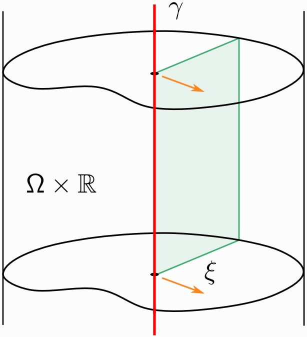

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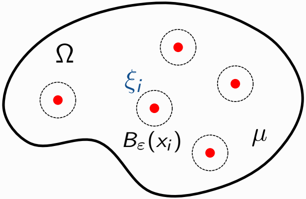

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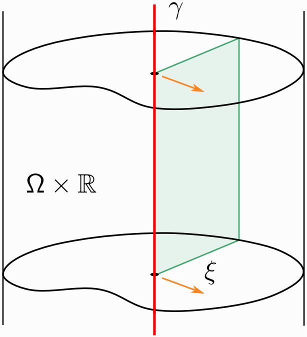

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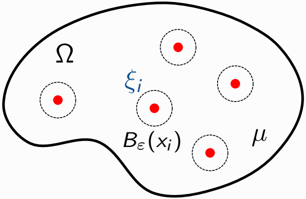

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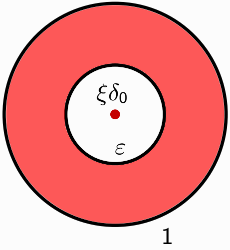

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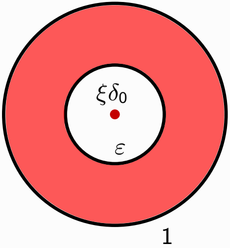

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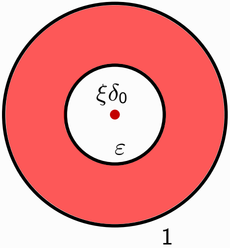

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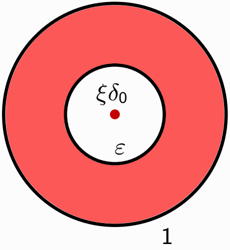

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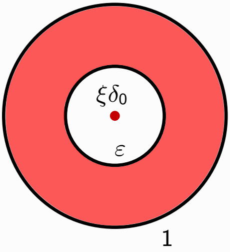

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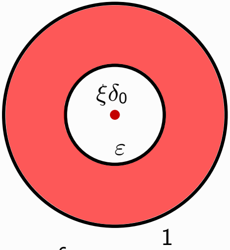

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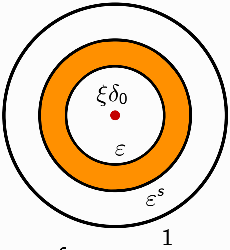

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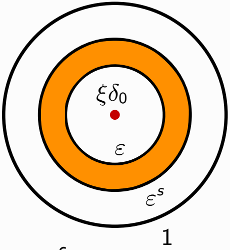

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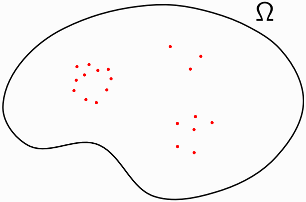

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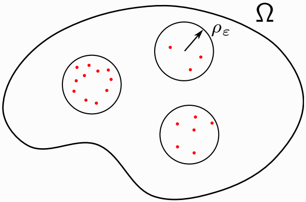

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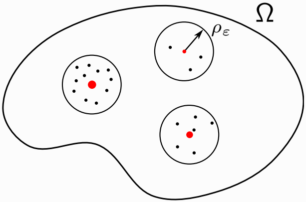

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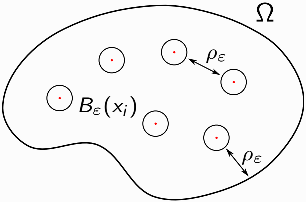

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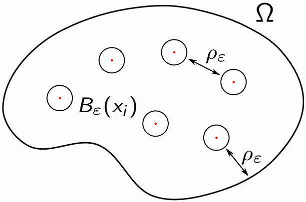

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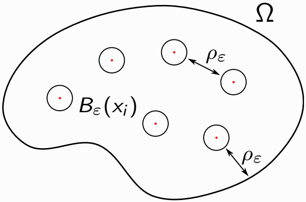

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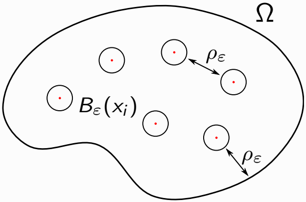

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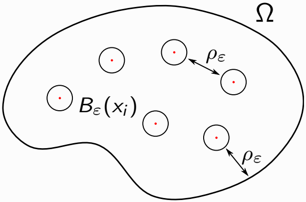

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  F., Palombaro, Ponsiglione. *Linearised Polycrystals from a 2D System of Edge Dislocations.* Preprint (2017)

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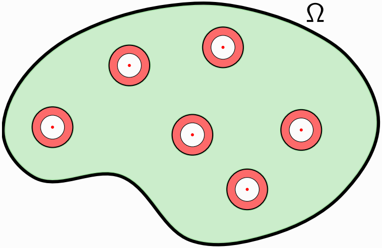

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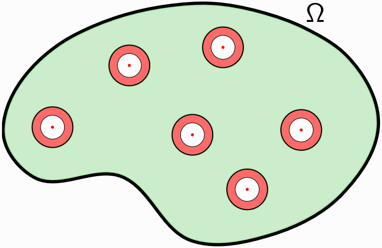

Idea: rescaling by $N_\varepsilon |\log \varepsilon|$, we have $E_\varepsilon^{\mathrm{interaction}} \to E^{\mathrm{elastic}}$ and $E_\varepsilon^{\mathrm{self}} \to E^{\mathrm{plastic}}$.

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

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- 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

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

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

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

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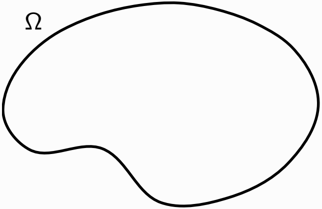

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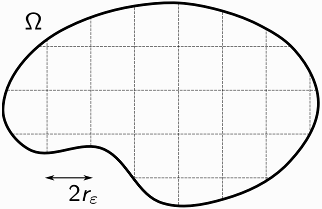

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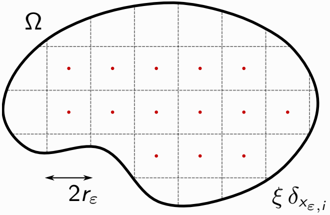

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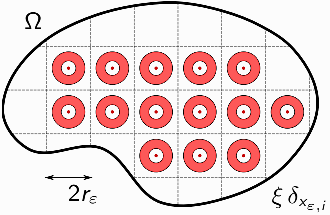

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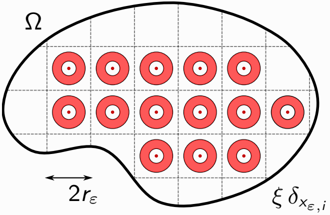

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$$\beta_\varepsilon = \sqrt{N_\varepsilon |\log \varepsilon|} S + N_\varepsilon A + K_\varepsilon + O(\sqrt{N_\varepsilon |\log \varepsilon|})$$

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.

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Theorem (F., Palombaro, Ponsiglione '17)

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 $\operatorname{Curl} A = \mu$ 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.

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

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

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Problem

Minimise

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

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Polycrystals as energy minimisers

Theorem (F., Palombaro, Ponsiglione '17)

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

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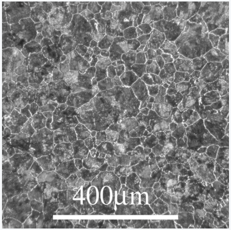
with $A_k \in \mathbb{M}^{2\times 2}_{\mathrm{skew}}$ *and* $\{E_k\}_{k=1}^{M}$ *Caccioppoli partition of* Ω. *We interpret* A *as a linearised polycrystal.*



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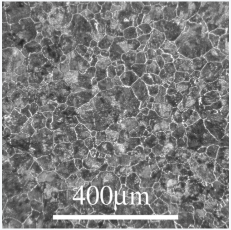

Proof Strategy: We are minimising an anisotropic total variation functional. By Coarea formula we select the levels with minimal perimeter, definying the Caccioppoli partition.

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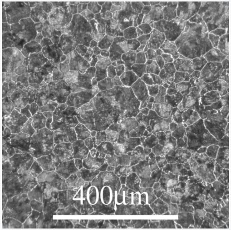

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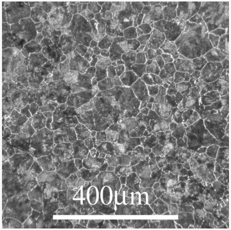

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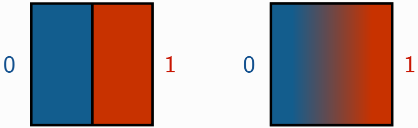

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  Namely, considering small deformations $v = x + \varepsilon u$. Now the Burgers vectors are $\varepsilon\xi$ and the equivalent rescaling is $\varepsilon^2 N_\varepsilon |\log\varepsilon|$.
  Müller, Scardia, Zeppieri. Indiana University Mathematics Journal (2014).

Thank You!