Variational approach to grain boundaries

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Wiki

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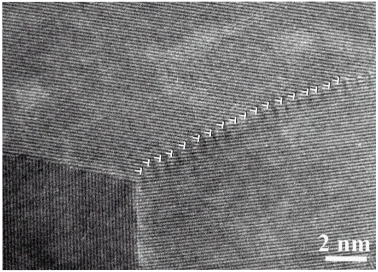
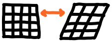


INTRODUCTION

- METALS ARE CRYSTALS

Elasticity

distorsion of an ordered structure



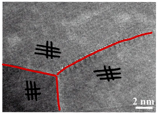
Plasticity

slips along "lattice preserving" directions

permant deform.

- CRYSTALS ARE LOCALLY ORDERED

→ POLYCRYSTALS



- REGIONS WITH DIFFERENT ORIENTATIONS ARE SEPARATED BY GRAIN BOUNDARIES

- INCOPATIBILITIES AT THE GRAIN BOUNDARIES INDUCE ELASTIC DISTORSION :

SURFACE TENSION

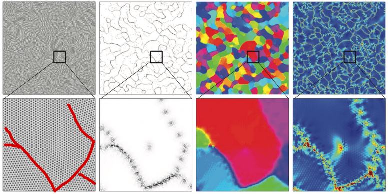
2D : grain boundary = curve γ

R_1 | R_2

γ

$R_i \in SO(2)$

rotation with respect to a reference configuration



Elsey - Wirth '15

ENERGY $\simeq \mathcal{H}^1(\gamma)$ (depends on the relative orientations)

- VARIATIONAL DERIVATION

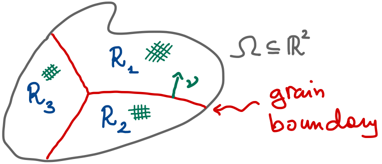
'Elastic energy' in the bulk $\leadsto$ 'surface tension' at grain boundaries

SHARP INTERFACE MODEL

SHARP INTERFACE MODEL FOR GRAIN BOUNDARIES

- **Configurations:**

  In each grain we see a constant rotation of a reference lattice



- **Energies:** Σ is the interface between grains

SURFACE TENSION

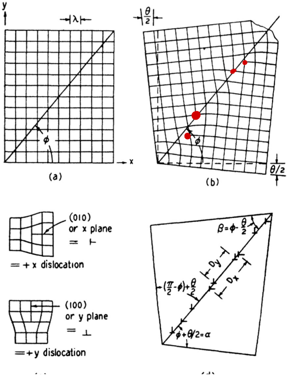
$$\int_{\Sigma} \varphi(R^+, R^-, \nu)\, d\mathcal{H}^1$$

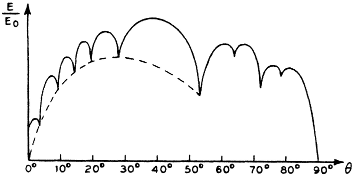
- $R(x)$ is the local orientation $R(x) = \sum_i R_i \chi_{E_i}(x)$
- $\{E_i\}$ is a partition of Ω

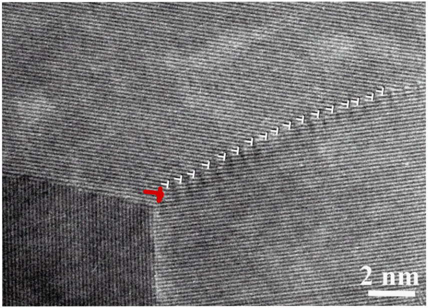
$$\text{Energy} = \sum_{ij} \mathcal{H}^1(\partial^* E_i \cap \partial^* E_j)\, \underbrace{\varphi(R_i, R_j, \nu_{ij})}_{\text{Energy per unit length}}$$

Q: what is the structure of the surface tension?

Read - Schockley





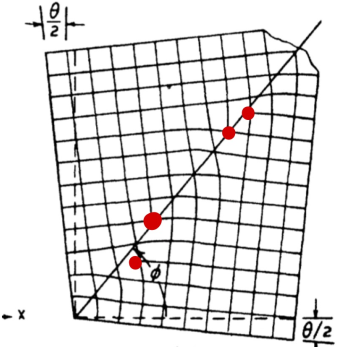


The interface energy is due to incompatibility

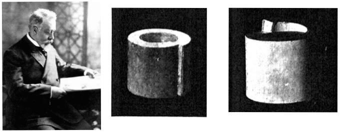
dislocations

$$E \simeq E_0\, \theta\, (|\log \theta| + 1)$$

Dislocations: defects in the lattice

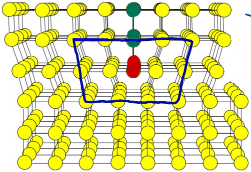


(b)

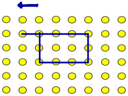


V. Volterra "Sur l'équilibre de corps élastiques..." 19

DISCRETE description



Burgers vector



Reference configuration

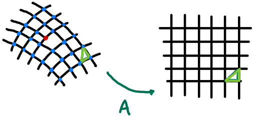
Burgers circuit

Core of the dislocation

Energy:

$\boxed{\text{Elastic energy outside the core}}$ + $\boxed{\text{core energy}}$

Lauteri-Luckhaus model



Dimension 2 $\quad \Omega \subseteq \mathbb{R}^2$

- $A : \Omega \to \mathbb{R}^{2\times 2}$ local deformation
- $S \subseteq \Omega$ s.t. $\operatorname{supp}[\operatorname{Curl} A] \subseteq S$ set of incompatibilities

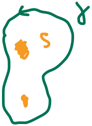
λε-neighborhood of set S

$$\boxed{E_\varepsilon(A,S) = \int_{\Omega \setminus B_{\lambda\varepsilon}(S)} \operatorname{dist}^2(A, SO(2))\,dx + |B_{\lambda\varepsilon}(S)|}$$

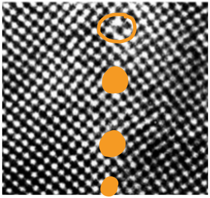
CONSTRAINTS: "QUANTIZATION OF CURL"

- If γ closed curve : $\gamma \cap S = \emptyset$

$$\Rightarrow \left| \int_\gamma A\cdot \tau \, ds \right| \geq \varepsilon \tau$$

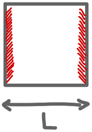
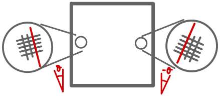


Ω



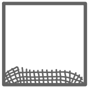
- $\tau > 0$ fixed
- $\varepsilon > 0$ "lattice spacing"

Heuristics:

$\min E_\varepsilon(A,S)$: $A = R_\theta$  $R_{-\theta}$ i.e. 

$$E_\varepsilon(A,S) = \int_{\Omega \setminus B_{\lambda\varepsilon}(S)} \mathrm{dist}^2(A, SO(2))\,dx + |B_{\lambda\varepsilon}(S)|$$

1) Elastic: $A = \nabla u$ $S = \emptyset$



$$E_\varepsilon(\nabla u, \emptyset) \simeq L^2$$

2) 'Sharp' transition $S = \{0\} \times [-1/2, 1/2]$

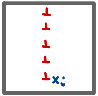
$A =$ 

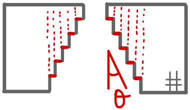
$$E_\varepsilon(A,S) = \lambda \varepsilon L$$

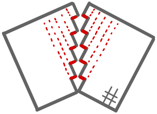
! scales as length

order ε

3) Insert defects $S = \{x_i\}$ $\mathrm{Curl}\, A = \sum_i \varepsilon b \delta_{x_i}$



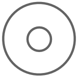




Energy of defects

$$\boxed{E_\varepsilon(A,S) = \int_{\Omega \setminus B_{\lambda\varepsilon}(S)} \mathrm{dist}^2(A, SO(2))\,dx + |B_{\lambda\varepsilon}(S)|}$$

- **One defect:** $\mathrm{Curl}\, A = \varepsilon b \delta_0$



$$\int_{B_r \setminus B_{\lambda\varepsilon}} \mathrm{dist}^2(A, SO(2))\,dx$$

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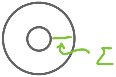

$A = \nabla w$

$$\int_{(B_r \setminus B_{\lambda\varepsilon}) \setminus \Sigma} \mathrm{dist}^2(A, SO(2))\,dx = \int_{B_r \setminus B_{\lambda\varepsilon}} \mathrm{dist}^2(\nabla w, SO(2))\,dx$$

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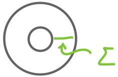
Rigidity FJM '02
$\exists R \in SO(2)$



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$$\geq C \int_{\lambda\varepsilon}^{r} \int_{\partial B_\rho} |(A-R)\cdot t|^2\, ds\, d\rho$$

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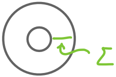

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$\boxed{\text{Jensen ineq.}}$

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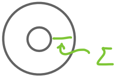

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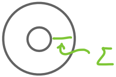

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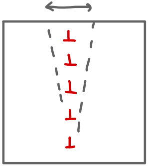
- **Array of defects for $\theta \ll 1$** : N defects

$N\varepsilon\tau \simeq L\theta$



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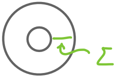

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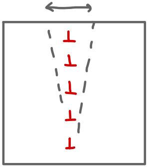

$$L/N \simeq \frac{\theta}{\varepsilon\tau}$$

Energy of defects

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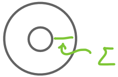

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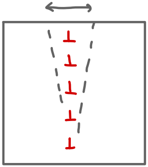


$$L/N \simeq \frac{\theta}{\varepsilon\tau}$$

$$\text{Energy} \simeq N\varepsilon^2\tau^2 \log\frac{\theta/\varepsilon\tau}{\lambda\varepsilon}$$

$$\simeq \varepsilon\tau L\theta\left[|\log\theta| + 1\right]$$

Read - Shockley

Main questions:

1. Is the model able to select minimizers that show grain boundaries?

2. The energy of grain boundaries does satisfy Read and Shockley formula?

3. Are minimizers given, as in the heuristics, by arrays of equidistributed defects?

4. Can we describe these results in the asymptotics as $\varepsilon \to 0$?

$$\boxed{F_\varepsilon(A,S) := \frac{1}{\varepsilon}\left[\int_{\Omega \setminus B_{\lambda\varepsilon}(S)} \mathrm{dist}^2(A,S)\,dx + |B_{\lambda\varepsilon}(S)|\right]}$$

SOME REFERENCES

↳ LARGE CLASS OF "SEMI-DISCRETE" MODELS

$$F_\varepsilon(A,S) := \frac{1}{\varepsilon}\left[\int_{\Omega\setminus B_{\lambda\varepsilon}(S)} \mathrm{dist}^2(A,S)\,dx + |B_{\lambda\varepsilon}(S)|\right]$$

↳ continuum approximation outside the core

MANY SIMILAR MODEL FOR DIFFERENT ENERGY REGIMES (DILUTE)

- Core radius
  - Ponsiglione, De Luca-AG-Ponsiglione, AG-Leoni-Ponsiglione (2d linear)
  - Scardia-Zeppieri, Muller-Scardia-Zeppieri (2d non linear)
  - Conti-AG-Ortiz, AG-Marziani-Scala - Conti-AG-Marziani (3d)

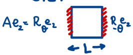
  Other: Ginster, ...
- Phase field model (Nabarro-Peierls)
  - Koslowski-Ortiz, AG-Muller, Cacace-AG, Conti-AG-Muller ...
- Discrete justifications/formulations
  - Ariza-Ortiz, Hudson-Ortner, Alicandro-De Luca-AG-Ponsiglione, Giuliani-Theil
  - Alicandro-De Luca-Lazzaroni-Palombaro-Ponsiglione ....
  - Mugnai-Luckhaus
- Related
  - Brezis-Bethuel-Hélein, Sandier-Serfaty, Jerrard (Ginzburg-Landau) ....
  - Cicalese-Ponsiglione (XY vs G-L vs dislocations) ....

LAUTERI-LUCKHAUS RESULT

Understanding configurations with small energy and justifying Read and Shockley formula....

upper bound
- construction

$$C_1 L\theta(|\log\theta|+1) \leq \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\inf_{\substack{b.c. \\ Q_L\setminus B_{\lambda\varepsilon}(S)}}\left[\int \mathrm{dist}^2(A,SO(2))\,dx + |B_{\lambda\varepsilon}(S)|\right] \leq C_2 L\theta(|\log\theta|+1)$$



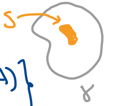
lower bound
- Many deep and powerfull ideas

Note: • The upper and lower bounds do not match

Q: • How robust is this model?

• Can all these ideas be used for other problems (discrete, clusters, ...)?

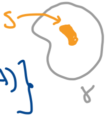
THEOREM (AG-Spadaro)



$$F_\varepsilon(A) = \frac{1}{\varepsilon} \inf \left\{ \int_{\Omega \setminus B_{\lambda\varepsilon}(S)} \mathrm{dist}^2(A, SO(2))\,dx + |B_{\lambda\varepsilon}(S)| \; : \; S \supseteq \mathrm{supp}\, \mathrm{Curl}(A) \right\}$$

$$\left| \int_\gamma A t \right| \geq r\varepsilon$$

THEOREM (AG-Spadaro)



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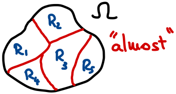
$$\left|\int_\gamma A t\right| \geq c\varepsilon$$

- **COMPACTNESS**

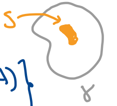
If $\sup F_\varepsilon(A_\varepsilon) < +\infty \Rightarrow \exists\, \varepsilon_n \to 0$ s.t.

- $A_{\varepsilon_n}\chi_{B_{\lambda\varepsilon_n}}(S_n) \xrightarrow[L^1]{} A$



- $\boxed{A \in SBV(\Omega, SO(2)) \qquad \nabla A = 0 \qquad \text{MICROROTATIONS}}$

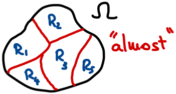
THEOREM (AG-Spadaro)



$$F_\varepsilon(A) = \frac{1}{\varepsilon} \inf \left\{ \int_{\Omega \setminus B_{\lambda\varepsilon}(S)} \mathrm{dist}^2(A, SO(2))\,dx + |B_{\lambda\varepsilon}(S)| \ : \ S \supseteq \mathrm{supp}\,\mathrm{Curl}(A) \right\}$$

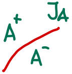
$$\left| \int_\gamma A t \right| \geq 2\varepsilon$$

- **COMPACTNESS**



If $\sup F_\varepsilon(A_\varepsilon) < +\infty \Rightarrow \exists\, \varepsilon_n \to 0$ s.t.

- $A_{\varepsilon_n} \chi_{B_{\lambda\varepsilon_n}}(S_n) \xrightarrow[L^1]{} A$
- $\boxed{A \in SBV(\Omega, SO(2)) \qquad \nabla A = 0 \qquad \text{MICROROTATIONS}}$

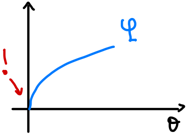


$\nabla A = 0$

$A \in SBV(\Omega, SO(2))$

- **GAMMA-CONVERGENCE**

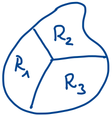
$$F_\varepsilon \xrightarrow[\Gamma(L^1)]{} F \qquad \boxed{F(A) = \int_{J_A} \varphi(|A^+ - A^-|)\, d\mathcal{H}^1}$$



$$\boxed{C_1 \theta(|\log\theta| + 1) \leq \varphi(\theta) \leq C_2 \theta(|\log\theta| + 1)}$$

REMARK ON COMPACTNESS :

$F_\varepsilon(A_\varepsilon) < M \implies$ up to a subseq. $A_\varepsilon \longmapsto A$



- Identify the class of fields with limiting finite energy

- Convergence of minimizers

Key ingredients :

- $\boxed{\text{Rigidity for incompatible fields}}$ (Muller-Scardia-Zeppieri)

$\forall A \in L^2(\Omega, \mathbb{R}^{2\times 2}) \quad \exists R \in SO(2)$

$$\int_\Omega |A-R|^2 dx \leq C\left[\int_\Omega \mathrm{dist}^2(A, SO(2))\,dx + |\mathrm{Curl}\,A|^2(\Omega)\right]$$

· AG-Ponsiglione (linear)

· Conti-AG $n \geq 3$

- $\boxed{\text{Lauteri-Luckhaus strategy}}$
  - Refinement of the sequence A_ε
  - Local lower (! very technical)

· $A_\varepsilon \rightsquigarrow \tilde{A}_\varepsilon \qquad \tilde{A}_\varepsilon \xrightarrow[L^1]{} A \in BV$

· $A \in SBV$
$\nabla A = 0$

CELL PROBLEM FORMULA

$$\Psi(|R_1 - R_2|) := \inf \left\{ \varliminf_{\varepsilon \to 0} F_\varepsilon(A_\varepsilon, Q_1) \ : \ A_\varepsilon \xrightarrow{L^1} I_{R_1,R_2} = \boxed{R_1 \mid R_2} \right\}$$

CELL PROBLEM FORMULA

$$\varphi(|R_1 - R_2|) := \inf \left\{ \lim_{\varepsilon \to 0} F_\varepsilon(A_\varepsilon, Q_1) \ : \ A_\varepsilon \xrightarrow{L^1} I_{R_1,R_2} = \boxed{R_1 \,|\, R_2} \right\}$$

$$\overset{!}{=} \lim_{\varepsilon \to 0} \inf \left\{ F_\varepsilon(A, Q_1) : \ \text{b.c} \quad A = I_{R_1 R_2} \text{ in } Q_1^c \right\}$$

To show ! is crucial

$$= \lim_{L \to +\infty} \frac{1}{L} \inf \left\{ F_1(A, Q_L) \ : \ \text{b.c.} \quad A = I_{R_1 R_2} \ Q_L^c \right\}$$

CELL PROBLEM FORMULA

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PROP

$$\exists \lim_{\varepsilon\to 0} \varphi_\varepsilon(R_1,R_2) = \lim_{L\to+\infty} \varphi_L(R_1,R_2) =: \varphi_\infty(R_1,R_2)$$

CELL PROBLEM FORMULA

$$\varphi(|R_1-R_2|) := \inf\left\{ \lim_{\varepsilon\to 0} F_\varepsilon(A_\varepsilon, Q_1) \ : \ A_\varepsilon \xrightarrow{L^1} I_{R_1,R_2} = \boxed{R_1 \mid R_2} \right\}$$

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To show ! is crucial

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PROP

$$\exists \lim_{\varepsilon\to 0} \varphi_\varepsilon(R_1,R_2) = \lim_{L\to+\infty} \varphi_L(R_1,R_2) =: \varphi_\infty(R_1,R_2) = \varphi_\infty(|R_1-R_2|)$$

invariance by rotations

Monotonicity formula
(up to small boundary errors)

$$\underset{L-L}{\Longrightarrow} \quad \varphi_\infty(\alpha) \simeq \alpha(|\log\alpha|+1)$$

Crucial result:

$\varphi(|R_1-R_2|) = \varphi_\infty(|R_1-R_2|)$

$$\inf\left\{ \lim_{\varepsilon\to 0} F_\varepsilon(A_\varepsilon, Q_1) \ : \ A_\varepsilon \xrightarrow{L^1} I_{R_1,R_2} = \boxed{R_1 \mid R_2} \right\} \overset{!}{=} \lim_{\varepsilon\to 0} \inf\left\{ F_\varepsilon(A, Q_1) : \ \text{b.c} \ \ A = I_{R_1 R_2} \text{ in } Q_1^c \right\}$$

proof of !

- ($\leq$) "easy" $\rightsquigarrow$ scaling argument $\Rightarrow$ $\varphi \leq \varphi_\infty$

Crucial result: $\varphi(|R_1-R_2|) = \varphi_\infty(|R_1-R_2|)$

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proof of !

- $(\leq)$ "easy" $\rightsquigarrow$ scaling argument $\Rightarrow$ $\varphi \leq \varphi_\infty$

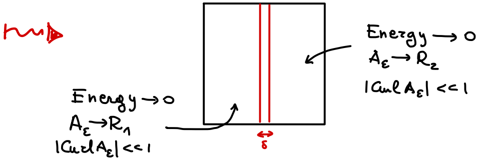
- $(\geq)$ Take A_ε optimal sequence, i.e. $F_\varepsilon(A_\varepsilon,Q_1) \to \varphi(|R_1-R_2|)$
  $A_\varepsilon \xrightarrow[L^1]{} I_{R_1,R_2}$

IMPORTANT: Need to change the boundary values !

- The classical "De Giorgi trick" of finding a section with small energy and using to make a cut-off is not immediate since A_ε is not a gradient

Changing the boundary conditions: part 1

- We choose an optimal sequence A_ε s.t.
    - $F_\varepsilon(A_\varepsilon, [-\delta,\delta]\times(-\frac{1}{2},\frac{1}{2})) \longrightarrow \varphi(|R_1 - R_2|)$



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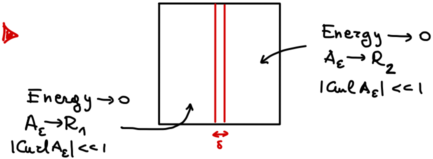
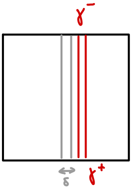
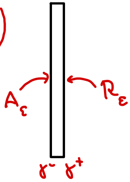


- Look for vertical section γ^- where A_ε is close to a rotation R_ε



$\Rightarrow$ connect elastically A_ε and R_ε

Important: The energy is scaled by $\frac{1}{\varepsilon}$!



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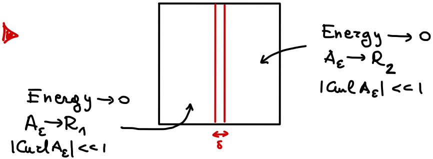

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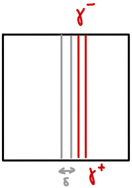

$\Longrightarrow$ connect elastically A_ε and R_ε

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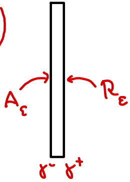
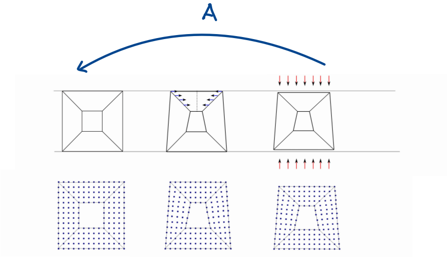


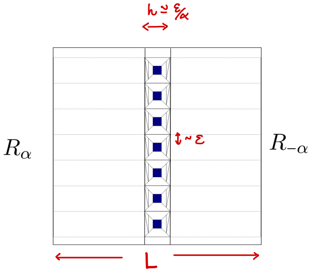
- If we connect elastically to a rotation R_ε (almost the right rotation)

  $\Longrightarrow$ we know how to connect rotations

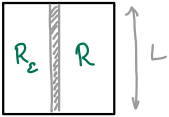
Changing the boundary conditions: part 2

L-L Construction for the upper bound





Energy $\simeq \alpha(|\log\alpha|+1)L$



<u>Note</u>: It also provides a way of connecting <u>two rotations</u> R_ε and R with an energy proportional to the interfaces and vanishing when $|R_\varepsilon - R| \to 0$

Changing the boundary conditions: part 3

Theorem:

If $F_\varepsilon(A_\varepsilon, Q_1) = \omega_\varepsilon \to 0$ and $A_\varepsilon \xrightarrow{L^1} R$

$\Rightarrow \; \exists \, \tilde{A}_\varepsilon$ s.t.

- $\tilde{A}_\varepsilon = A_\varepsilon$ on 
- $\tilde{A}_\varepsilon = R$ on 
- $F_\varepsilon(\tilde{A}_\varepsilon, Q_1) \to 0$

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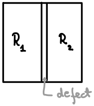
$\exists\, \tilde A_\varepsilon$ optimal sequence

$F_\varepsilon(\tilde A_\varepsilon,Q_1)\to\varphi(|R_1-R_2|)$

$\tilde A_\varepsilon =$ 

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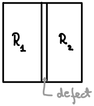
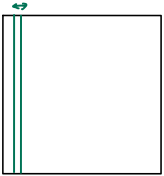
$\tilde{A}_\varepsilon =$ 

1) Find a stripe with small energy and small cut



$\ell = \sqrt{\frac{\varepsilon}{\omega_\varepsilon}}$

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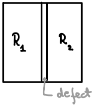
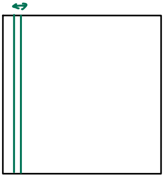
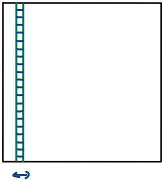
$\tilde{A}_\varepsilon =$ 

1) Find a stripe with small energy and small curl



$\ell = \sqrt{\frac{\varepsilon}{\omega_\varepsilon}}$

2) Divide in squares where apply rigidity



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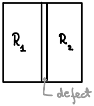
$\tilde{A}_\varepsilon =$ 

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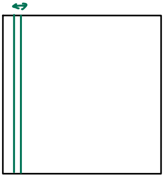

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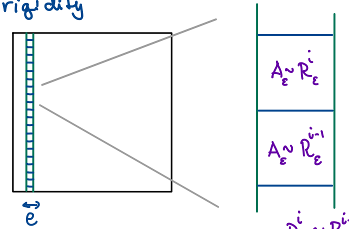

$R^i_\varepsilon \sim R^{i-1}_\varepsilon \sim R$

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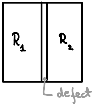
$\tilde A_\varepsilon =$ 

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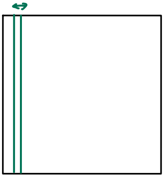

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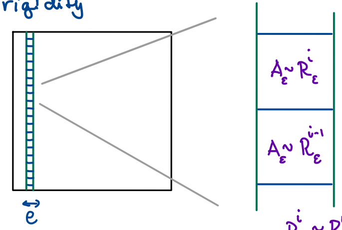
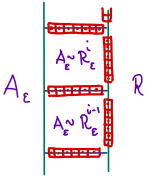
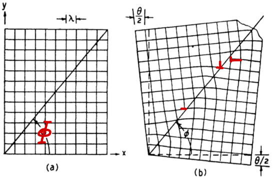


$R^i_\varepsilon \sim R^{i-1}_\varepsilon \sim R$

4) Connect rotations using small energy and elastically connect A_ε to rotations



GENERALIZATIONS: MORE REALISTIC ANISOTROPIC INTERFACE ENERGY



Read - Shockley

Energy of interface $\simeq [\cos\phi + \sin\phi]\,\theta\,(|\log\theta| + 1)$

Change the constraint on the circulation :

(Fortuna - AG - Spadaro . in preparation)

- $A : \Omega \longrightarrow \mathbb{R}^{2\times 2}$
- $S \supset \operatorname{supp} \operatorname{Curl} A$
- $\boxed{\int_\gamma A\cdot t \in \varepsilon \mathbb{Z}^2}$

$\mapsto \varphi(R_1, R_2, \nu)$

normal to the interface

Key ingredient: Construction for the cell pb. formula

CONCLUSIONS

- Lauteri-Luckhaus model (and method) is very robust
- It provides a derivation of a physically meaningfull model for grain boundaries
- It is a good lower bound for other models:
  - Partition pb $\longrightarrow$ compactness + cost of interphases
  - Other discrete model that show local order and allow for defects

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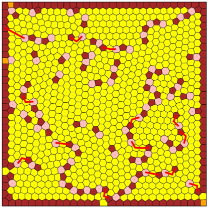
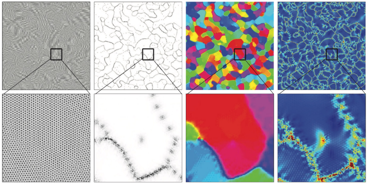


- Del Nin, PhD Thesis (Partition probeems with b.c / clusters)
- Caglioti-Iacobelli-Golse (quantization of measures $\to$ transport)
- D. Bourne-Peletier-Theil '14

  (Work in progress: Alberti-Del Nin-AG-Spadaro)

Work in progress: Crismale-AG-Malusa
(Ambrosio-Tortorelli type approximation)



Elsey-Wirth '15 (polycrystal image reconstruction)

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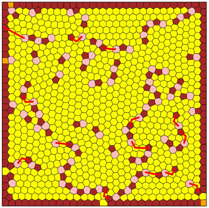

THANK YOU!

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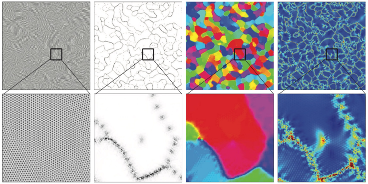

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