A line tension approximation for dislocations

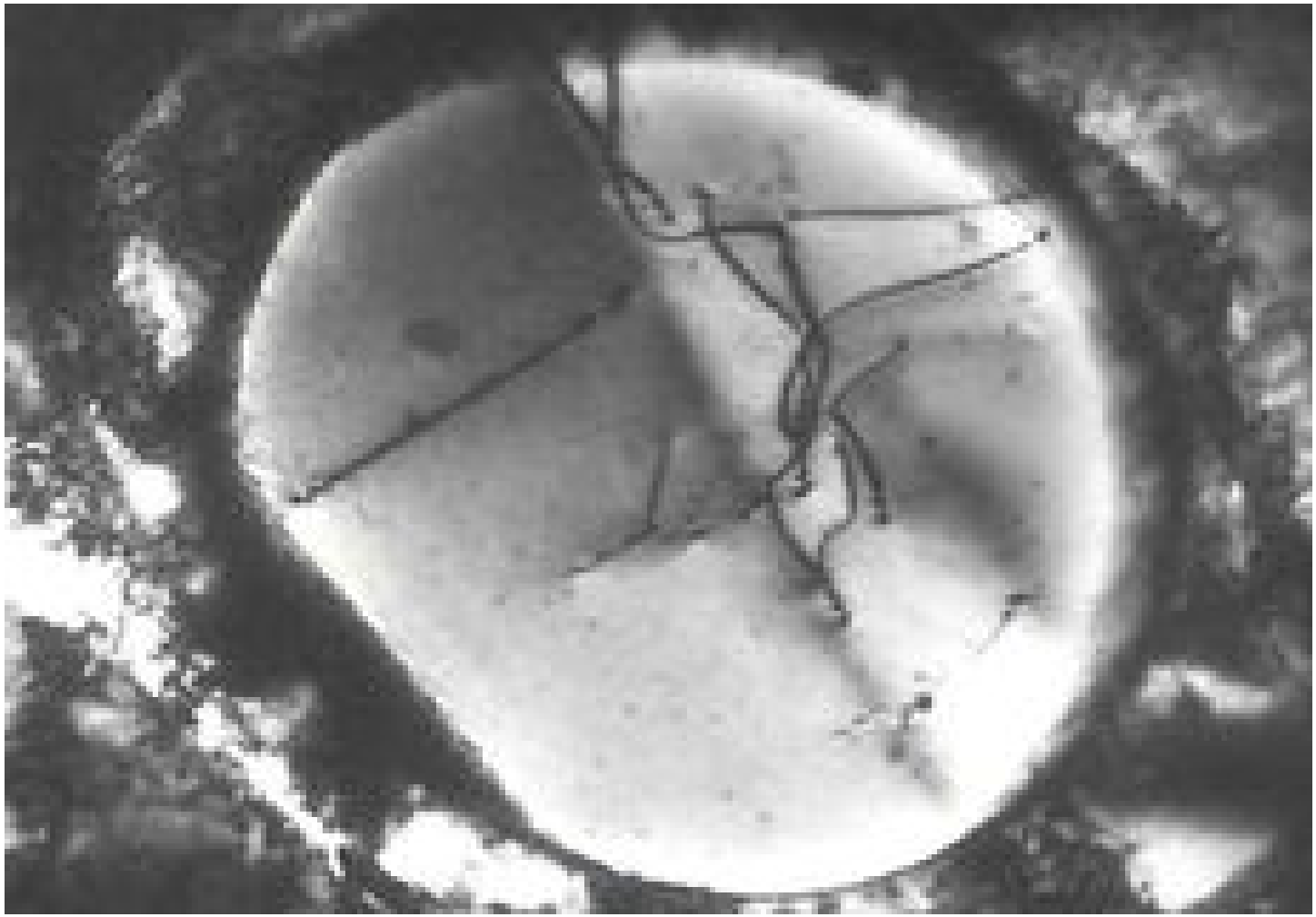
Adriana Garroni

Sapienza, Università di Roma

Mathematical Models for Dislocations
Rome, 13 December, 2007

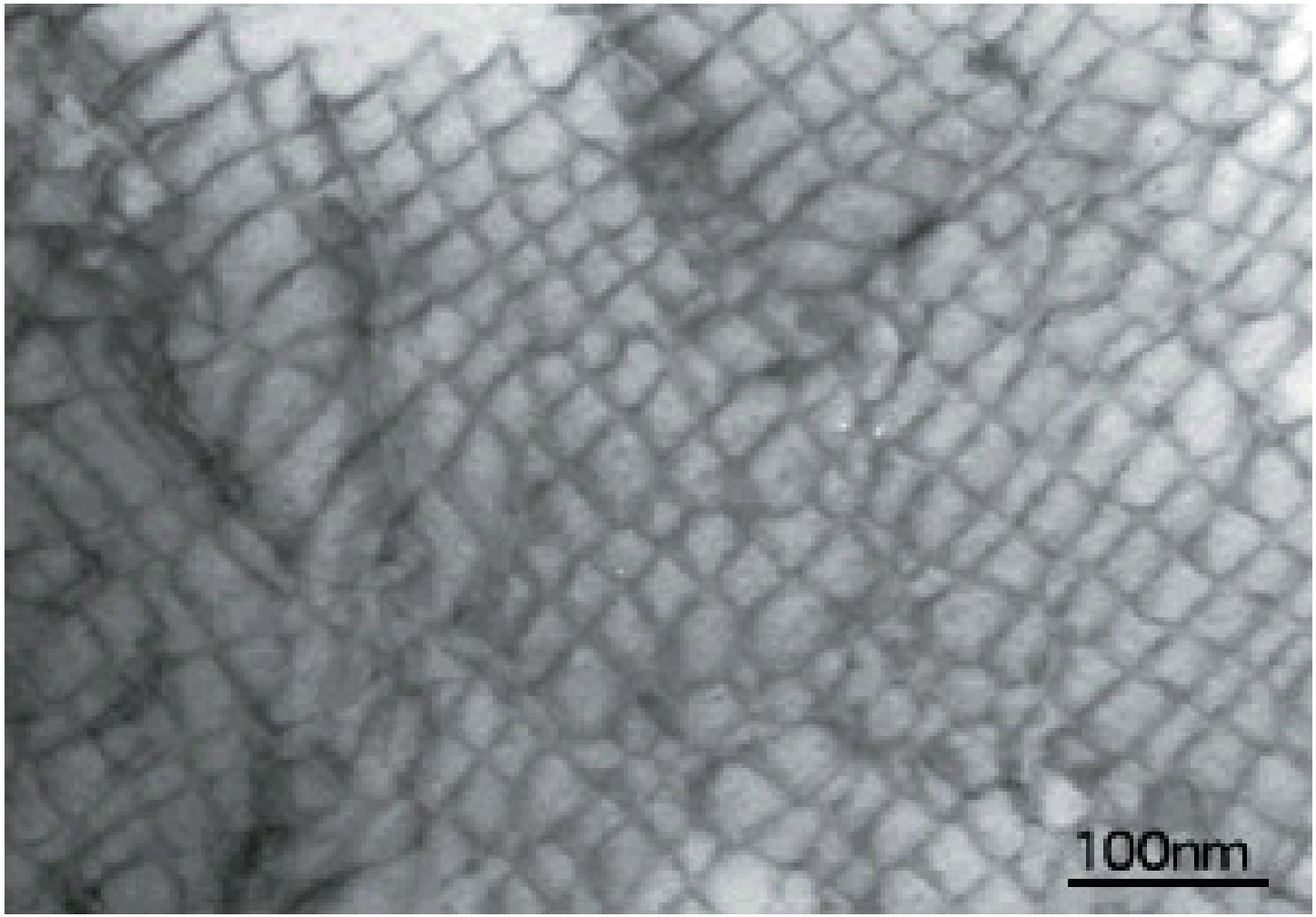
Single lines

Transmission Electron Micrograph of single Dislocations



Collective behaviour

Networks of dislocations



Collective behaviour: Formation of Microstructure

We believe that these configurations can be described asymptotically as equilibria of suitable Variational Models.

The general idea is that some of the traditional variational phenomenological models for dislocations can be improved starting from more fundamental models (first principles that account for the crystalline structure).

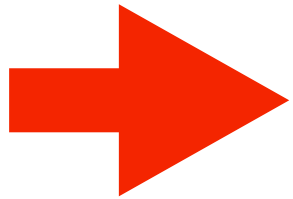
As a result we may obtain "unstable variational models", more precisely models that require relaxation and can explain the formation of microstructure.

Main goals of the project:

$3D$ discrete models

- Ariza and Ortiz, ARMA 2005

(Carpio and Bonilla, PRL 2003, PRB 2005)



Mesoscopic $3D$ model

- Concentration on lines

Macroscopic 3D model

- Plasticity

Crystal ANISOTROPY

Various collaborations (in chronological order)

S. Müller, M. Ortiz , P. Cermelli, G. Leoni, M. Focardi, S. Cacace , M. Ponsiglione, S. Conti

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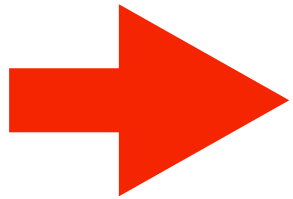

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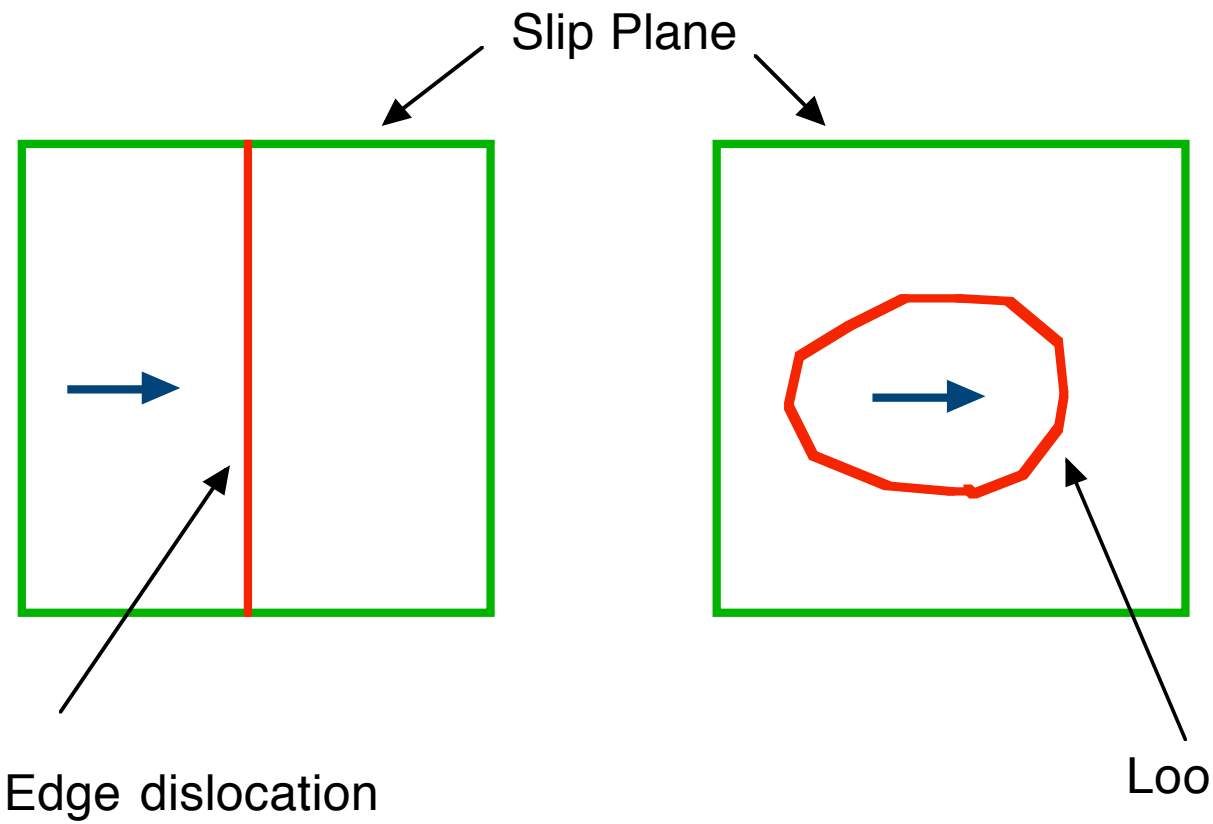
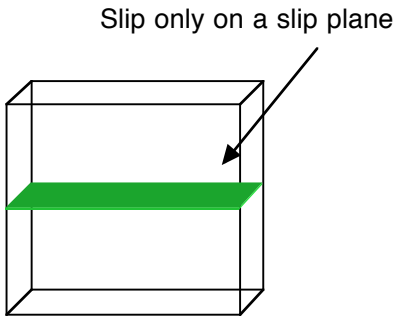


The dislocations are discontinuity of a phase field (the slip) on the slip plane

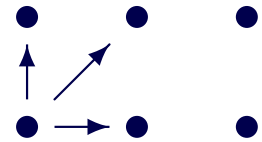
2D VARIATIONAL MODEL

(Koslowski-Ortiz/ Nabarro-Peierls)



$$Q = (0,1)^2 \subseteq \mathbb{R}^2$$

$$\text{Slip} \quad = \quad u : Q \to \mathbb{R}^2 \quad \text{(Unknown)}$$



$$E_{\text{tot}}(u) \quad = \quad E_{\text{elast.}}(u) \quad + \quad E_{\text{interface}}(u)$$

$E_{\text{elast.}}(u)$: Long-range elastic energy induced by the slip

$E_{\text{interface}}(u)$: Interfacial energy that penalizes slips not compatible with the lattice

$$\int_Q \int_Q (u(x)-u(y))^t \mathbf{\Gamma}(x-y)(u(x)-u(y))\,dx\,dy + \frac{1}{\varepsilon}\int_Q \text{dist}^2\,(u,\mathbb{Z}^2)\,dx$$

$\mathbf{\Gamma}$ is a matrix valued singular kernel

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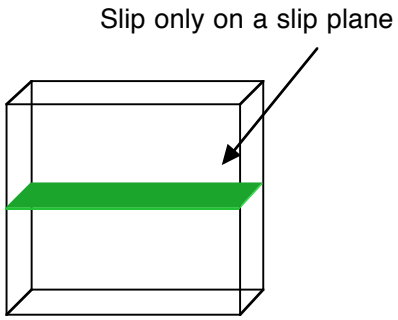

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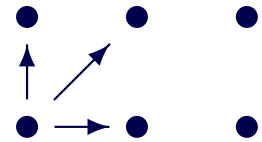

$$E_{\text{tot}}(u) \quad = \quad E_{\text{elast.}}(u) \quad + \quad E_{\text{interface}}(u)$$

ε = small parameter
$\sim$ lattice spacing

Long-range elastic energy induced by the slip

Interfacial energy that penalizes slips not compatible with the lattice

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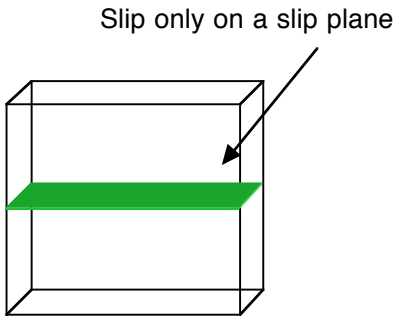

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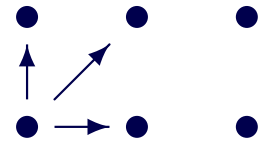

$$E_\varepsilon(u) = E_{\text{tot}}(u) \quad = \quad E_{\text{elast.}}(u) \quad + \quad E_{\text{interface}}(u)$$

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Long-range elastic energy induced by the slip

Interfacial energy that penalizes slips not compatible with the lattice

$$\int_Q \int_Q (u(x)-u(y))^t \mathbf{\Gamma}(x-y)(u(x)-u(y))\,dx\,dy + \frac{1}{\varepsilon}\int_Q \text{dist}^2\,(u,\mathbb{Z}^2)\,dx$$

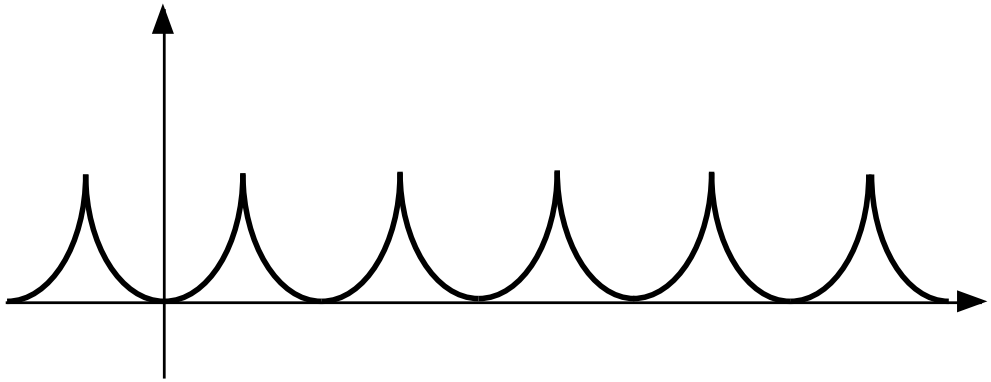
$\mathbf{\Gamma}$ is a matrix valued singular kernel

The interfacial Energy

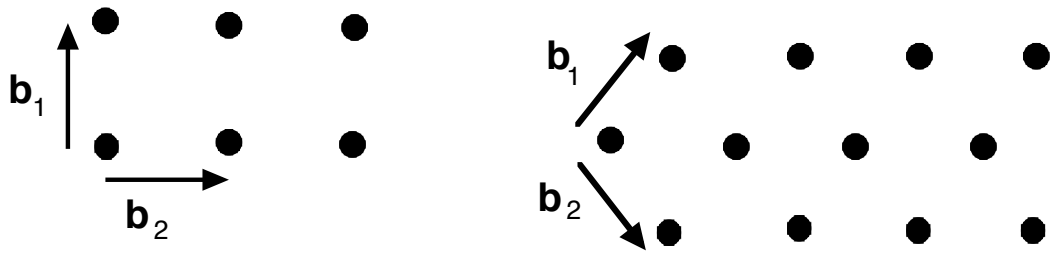
We write u in a basis given by two normalized Burgers vectors

$$u = u_1 \mathbf{b}_1 + u_2 \mathbf{b}_2$$

$$E_{\text{interface}}(u) = \frac{1}{\varepsilon} \int_Q \operatorname{dist}^2 (u, \mathbb{Z}^2)\, dx$$



Note: The Burgers vectors are determined by the crystalline structure



The Long-Range Elastic Interaction

NOTE: In order to understand the properties of the singular kernel, consider the following elementary example

$$\pi \min_{v|_{x_3=0}=u} \int_{\mathbb{R}^3_+} |\nabla v|^2 dx = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \frac{|u(x)-u(y)|^2}{|x-y|^3} dx\, dy =: [u]_{H^{\frac{1}{2}}}$$

Similarly the term $E_{\text{elast.}}(u)$ is obtained minimizing the bulk elastic energy given the slip on $\{x_3 = 0\}$

$$E_{\text{elast.}}(u) = \int_Q \int_Q (u(x)-u(y))^t \mathbf{\Gamma}(x-y)(u(x)-u(y))\, dx\, dy$$

Then: $\mathbf{\Gamma}(t) \in \mathbb{M}^{2\times 2}$

- $\frac{c_1}{|t|^3}|\xi|^2 \leq \xi^T \mathbf{\Gamma}(t)\xi \leq \frac{c_2}{|t|^3}|\xi|^2$ $\quad H^{\frac{1}{2}}$-type of kernel
- Fore simplicity we assume $\mathbf{\Gamma}(\lambda t) = |\lambda|^{-3}\mathbf{\Gamma}(t)$

Note: The precise structure of $\mathbf{\Gamma}$ depends on the boundary conditions and the crystalline structure

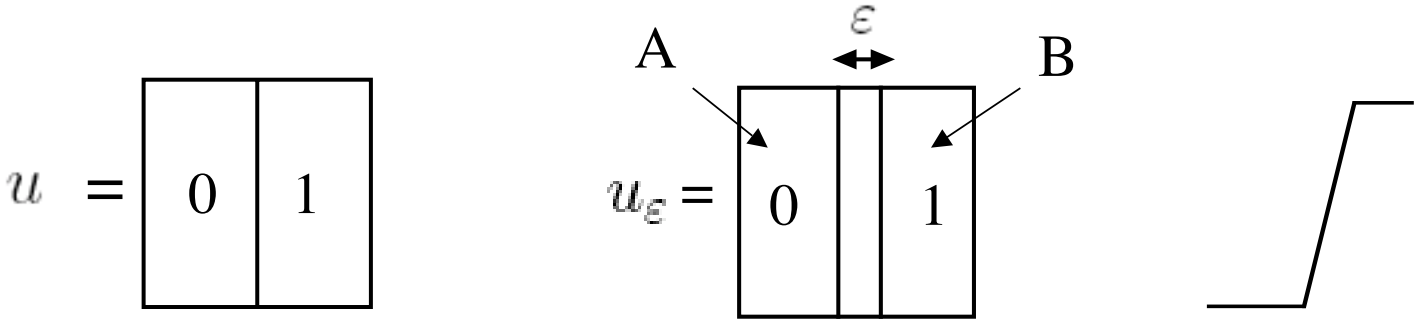
Main Goal

To study the asymptotic behaviour in terms of Γ-convergence of

$$E_\varepsilon(u) = \int_Q\int_Q (u(x)-u(y))^t \mathbf{\Gamma}(x-y)(u(x)-u(y))\,dx\,dy + \frac{1}{\varepsilon}\int_Q \mathrm{dist}^2\,(u,\mathbb{Z}^2)\,dx$$

properly scaled

1. The scaling: How much does it "cost" a jump with the $H^{\frac{1}{2}}$ norm?



$$E_\varepsilon(u_\varepsilon) \sim \int_Q\int_Q \frac{|u_\varepsilon(x)-u_\varepsilon(y)|^2}{|x-y|^3}\,dx\,dy \;+\; \text{l.o.t.}$$

$$= \int_A\int_B \frac{|u_\varepsilon(x)-u_\varepsilon(y)|^2}{|x-y|^3}\,dx\,dy \;+\; \text{l.o.t.} = \; C|\log\varepsilon| \;+\; \text{l.o.t.}$$

Γ-convergence of the functional

$$F_\varepsilon(u) = \frac{1}{|\log\varepsilon|}\int_Q\int_Q (u(x)-u(y))^t \mathbf{\Gamma}(x-y)(u(x)-u(y))\,dx\,dy + \frac{1}{\varepsilon|\log\varepsilon|}\int_Q \mathrm{dist}^2\,(u,\mathbb{Z}^2)\,dx$$

This is a multiple well potential with a singular perturbation (non local, singular and anisotropic): sharp interface limit.

A short list of references:

- (local perturbation)
  - Modica-Mortola, Modica, Sternberg, Bouchitte .....
- (non local, regular perturbation)
  - Alberti-Bellettini, Alberti-Bellettini-Cassandro-Presutti (Ising)
- (non local, singular perturbation)
  - Alberti-Bouchitte-Sepeccher, Kurzke, G.-Muller, Cacace-G.

Two words about Γ-convergence
(Cleverly designed the get convergence of minimum problems)

MAIN POINT:
given F_ε we replace it with a simpler functional F (no dependence on the small parameter ε!) that captures the main features of F_ε.

Essentially $F(u)$ is the smallest value that you reach with $F_\varepsilon(u_\varepsilon)$ among all sequences converging to u.

Usual strategy:
get a LOWER BOUND for $F_\varepsilon(u_\varepsilon)$ and then proof its OPTIMALITY.

Theorem

(Cacace-G.)

(Compactness)

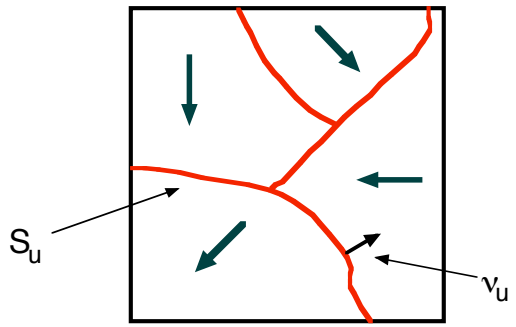
If $F_\varepsilon(u_\varepsilon) \leq C$, then (up to a subsequence) $\exists\ a_\varepsilon \in \mathbb{Z}^2$ and $u \in BV(Q, \mathbb{Z}^2)$ such that

$$u_\varepsilon - a_\varepsilon \to u \quad \text{in} \quad L^p \qquad \forall p < 2$$

(Γ-convergence)

$\exists$ a subsequence $\varepsilon_k \to 0$ and a function $\varphi : \mathbb{Z}^2 \times S^1 \to \mathbb{R}$ such that

$$F_{\varepsilon_k}(u) \quad \Gamma\text{-converges to } F(u) = \int_{S_u} \varphi([u], \nu_u)\mathcal{H}^1$$



S_u= jump set of u
$[u]$ = jump of u
ν_u = normal vector on S_u

Anisotropic line tension energy

$$\int_{S_u} \varphi([u], \nu_u) d\mathcal{H}^1$$

NOTE: The proof of the Γ-convergence is based on an abstract argument: Compactness of Γ-convergence and integral representation of the limit.

Incomplete description

- ε_k: we extract a subsequence (we aspect that the whole sequence should converge)
- $\varphi =?$: we would like to characterize the line tension energy density

The problem is completely solved in the scalar case.

The scalar case

Only one slip system; i.e.

$$\text{slip} \quad = \quad u\mathbf{b}$$

where $u : Q \to \mathbb{R}$ is scalar and $\mathbf{b}$ is a given Burgers vector.
The functional reduces to

$$F_\varepsilon(u) = \frac{1}{|\log \varepsilon|} \int_Q \int_Q \Gamma(x-y)|u(x)-u(y)|^2 \, dx \, dy + \frac{1}{\varepsilon |\log \varepsilon|} \int_Q \mathrm{dist}^2 (u, \mathbb{Z}) \, dx$$

(Γ is a scalar kernel with the same singularity).

Theorem (G.-Müller, ARMA)

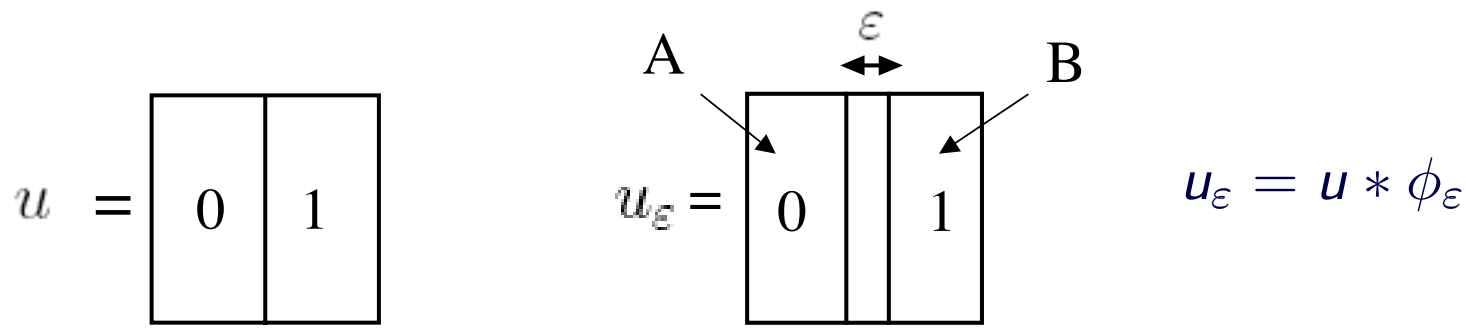
$$F_\varepsilon(u) \quad \Gamma\text{-converges to } F(u) = \int_{S_u} \gamma(\nu_u)|[u]|\mathcal{H}^1$$

where

$$\gamma(n) = 2 \int_{x \cdot n = 1} \Gamma(x) \, dx$$

Lower bound: For every sequence $u_\varepsilon \to u$ we prove that $\liminf_\varepsilon F_\varepsilon(u_\varepsilon) \geq F(u)$ (by a blow up argument)

Upper bound: The lower bound is achieved



$$\lim_\varepsilon F_\varepsilon(u_\varepsilon) = \lim_\varepsilon \frac{1}{|\log \varepsilon|} \int_Q \int_Q \Gamma(x-y)|u_\varepsilon(x)-u_\varepsilon(y)|^2 \, dx \, dy = \gamma(\mathbf{e}_1) = F(u)$$

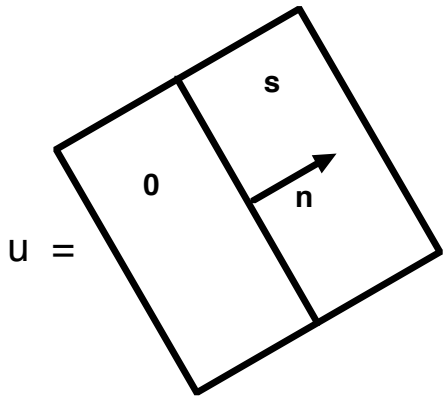
REMARK:

- Flat interface ("one-dimensional profile")
- The limit energy comes only from the non local part ("no equipartition of energy")

Back to the vector case

$$F_\varepsilon(u) = \frac{1}{|\log\varepsilon|}\int_Q\int_Q (u(x)-u(y))^t \Gamma(x-y)(u(x)-u(y))\,dx\,dy + \frac{1}{\varepsilon|\log\varepsilon|}\int_Q \mathrm{dist}^2\,(u,\mathbb{Z}^2)\,dx$$

Let us use naively the same strategy and for any $s \in \mathbb{Z}^2$ and $n \in S^1$ consider



$$u_\varepsilon = u * \phi_\varepsilon$$

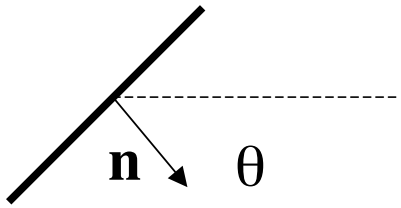
$$\lim_\varepsilon F_\varepsilon(u_\varepsilon) = s^t\gamma(n)s =: F_{\mathrm{flat}}(u)$$

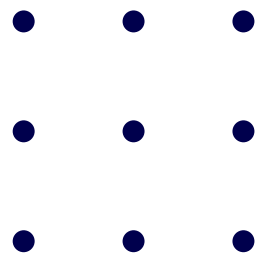
where

$$\gamma(n) = 2\int_{x\cdot n=1} \Gamma(x)\,dx = \begin{pmatrix} \gamma_{11}(n) & \gamma_{12}(n) \\ \gamma_{12}(n) & \gamma_{22}(n) \end{pmatrix}$$

NOTE: In general $F(u) < F_{\mathrm{flat}}(u)$.

EXAMPLE: CUBIC LATTICE





$$\gamma(n) = \gamma(\theta) = C \begin{pmatrix} 2(1 - \frac{1}{2}\cos^2\theta) & \frac{1}{2}\sin 2\theta \\ \frac{1}{2}\sin 2\theta & 2(1 - \frac{1}{2}\sin^2\theta) \end{pmatrix}$$

NOTE: The off-diagonal term is negative if $\theta < 0$

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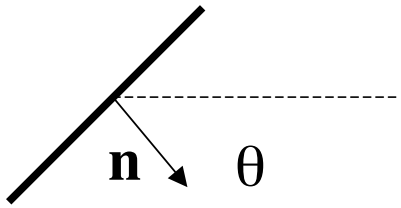

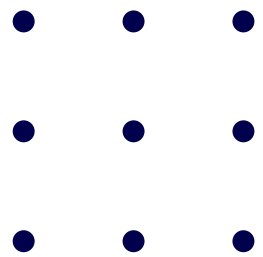

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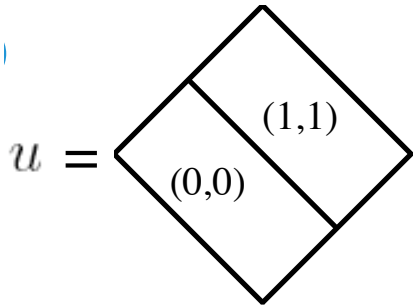
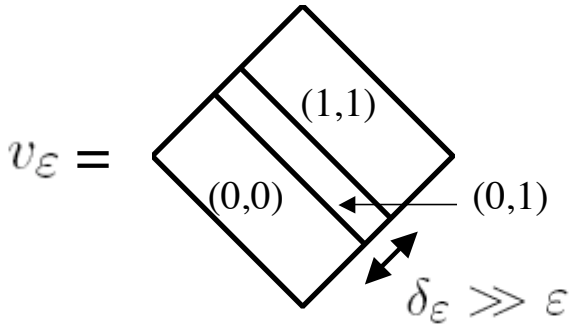
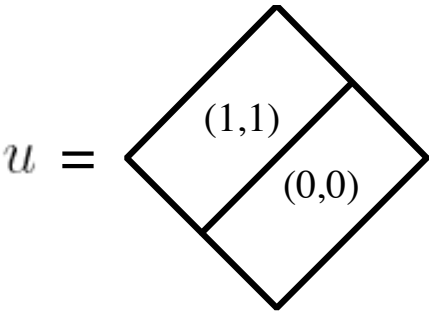
Important consequences

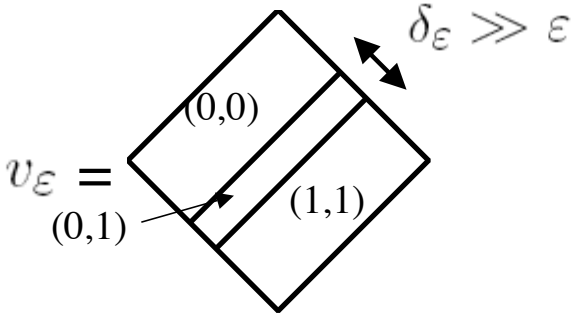
1. In some directions it is better to concentrate the jump





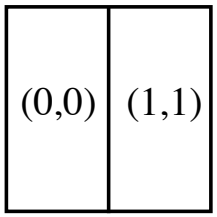
$$\lim_{\varepsilon \to 0} F_\varepsilon(u * \phi_\varepsilon) > \lim_{\varepsilon \to 0} F_\varepsilon(v_\varepsilon * \phi_\varepsilon)$$





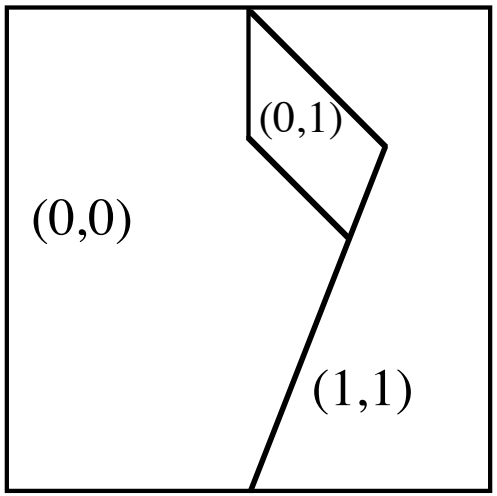
$$\lim_{\varepsilon \to 0} F_\varepsilon(u * \phi_\varepsilon) < \lim_{\varepsilon \to 0} F_\varepsilon(v_\varepsilon * \phi_\varepsilon)$$

2. NO "one dimensional" optimal profile

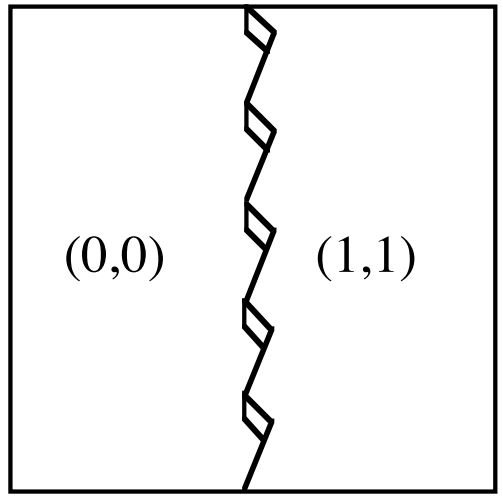
$u_0 =$ 

$$F_{\text{flat}}(u_0) := \lim_{\varepsilon} F_\varepsilon(u_0 * \phi_\varepsilon) = \gamma_{11}(\mathbf{e}_1) + \gamma_{22}(\mathbf{e}_2)$$

Consider

$v_\cdot =$ 

$\lim_{\delta \to 0} v_\delta = u_0$

$v_\delta =$ 

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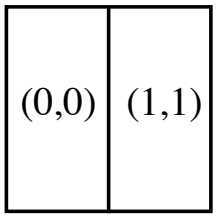
$u_0 =$ 

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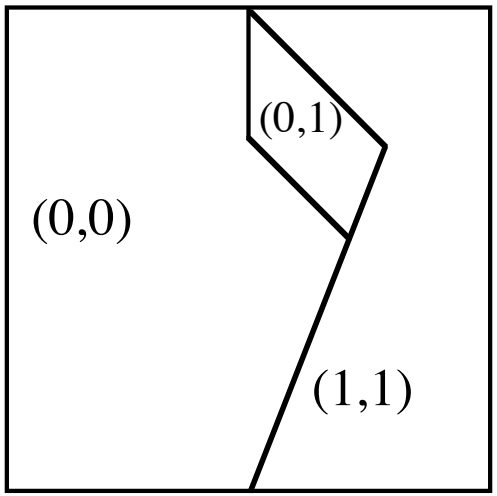
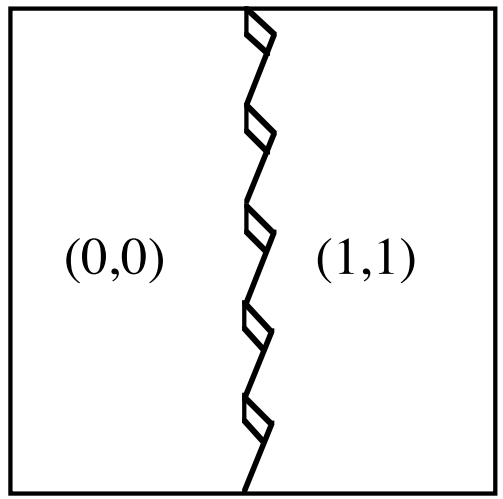
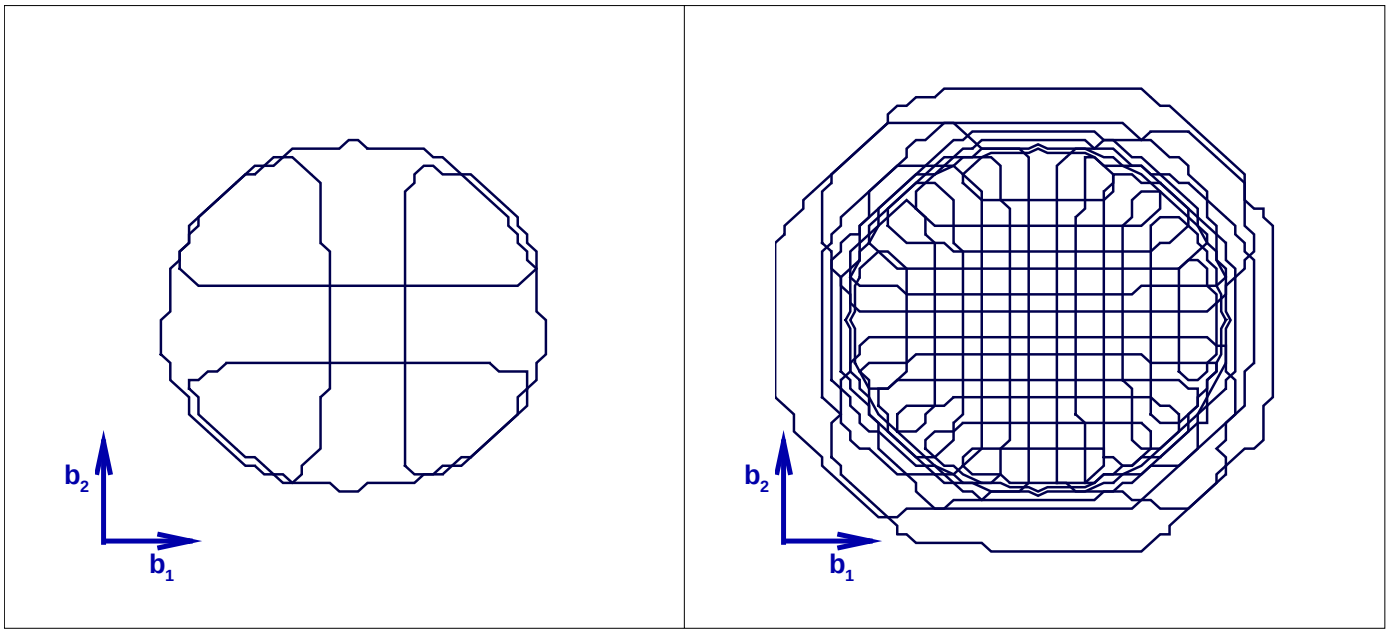
$v_\cdot =$ 

$v_\delta =$ 

$\lim_{\delta \to 0} v_\delta = u_0$

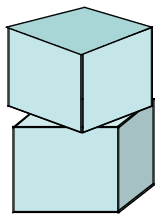
$$F_{\text{zig-zag}}(u_0) := \lim_{\varepsilon \to 0} F_\varepsilon(v_{\delta_\varepsilon} * \phi_\varepsilon) < F_{\text{flat}}(u_0)$$

Numerical simulations for a twist boundary problem using this model (Koslowki - Ortiz, 2004)

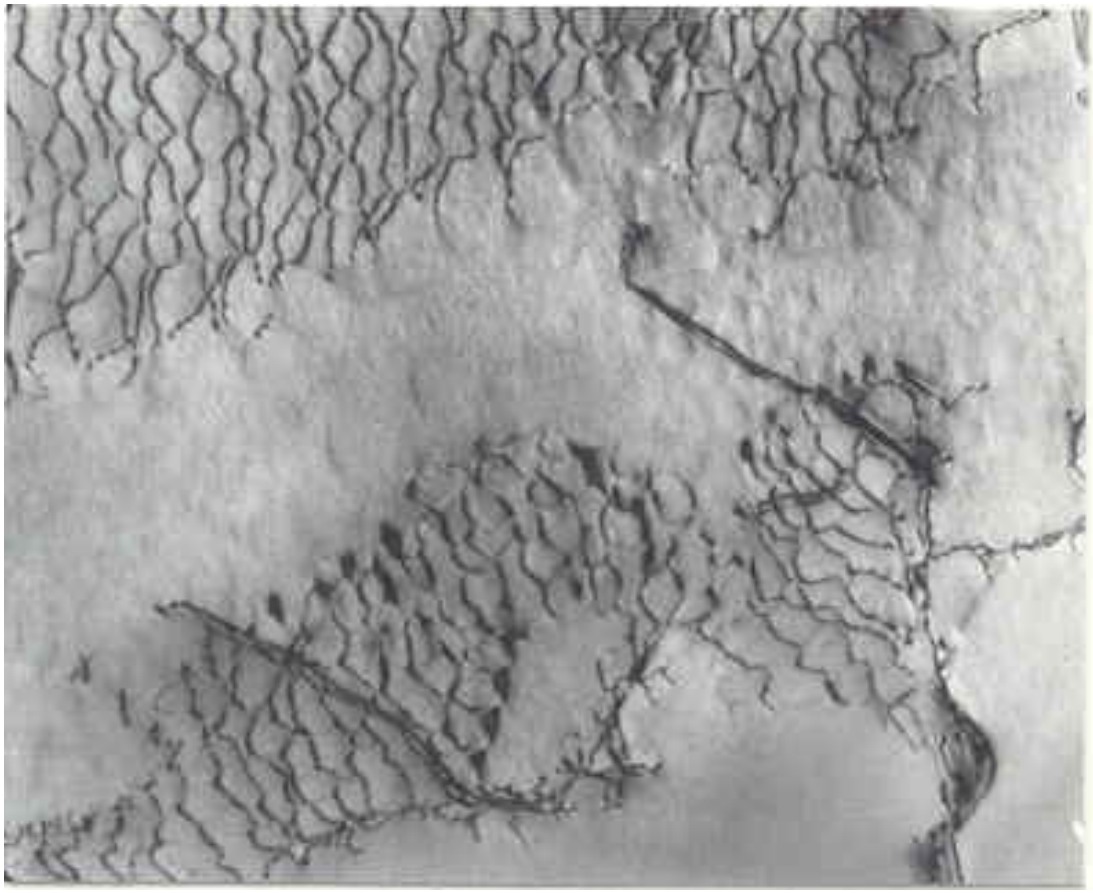


(a) $\theta = 0.01$ (b) $\theta = 0.05$

A twist of the upper part of the crystal wrt the lower part is imposed by requiring the constraint that the slip u be close to a given rotation of angle θ



Zig-Zag's of screw and edge dislocations observed at the TEM



Reasons for the formation of Microstructures

The naive line tension energy

$$F_{\text{flat}}(u) = \int_{S_u} [u]^t \gamma(n_u)[u] d\mathcal{H}^1$$

is NOT LOWER SEMICONTINUOUS

It requires relaxation: find the largest $\varphi(s,\nu) \leq s^t\gamma(\nu)s$ such that

$$\int_{S_u} \varphi([u], n_u)\, d\mathcal{H}^1$$

is lower semicontinuous.
We can prove (A.G., S. Conti, S. Müller) that this is exactly "zig-zag" energy (so our example gives the relaxation of F_{flat}) and we (almost) prove that the realaxation is the Γ-limit in the vector case.

CONCLUSIONS:

1. The anisotropic line tension energy is completely determined by the elastic tensors and the crystalline structure
   $\longrightarrow$ the whole sequence converges
2. The anisotropic line tension energy is given by a relaxation process
   $\longrightarrow$ microstructures
3. This final result is very technical already in the $2D$ case and suggests new difficulties in in the passage to the $3D$ case, but also that the $3D$ case could be very rich and may exhibit very interesting microstructures