

Multiscale problems in dislocation theory

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PLAN OF THE COURSE

- Part I: Preliminaries on dislocations
- Part II: Upscaling of dislocation energies
- Part III: Upscaling of dislocation evolutions
- Part IV: Equilibrium patterns of dislocations
- Part V: Equilibrium patterns of dislocations and beyond

PART I

Preliminaries on dislocations

Crystallographic structure

Atomic configurations in metals are generally **crystalline**.

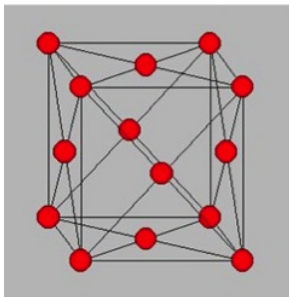
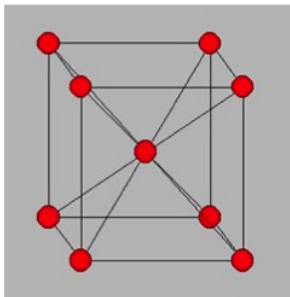
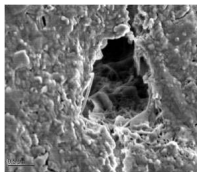
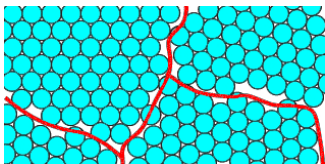
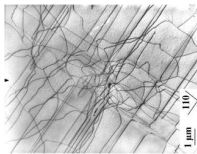
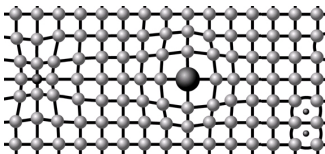


Figure: BCC and FCC crystals.

Crystallographic defects

There is no such thing as a perfect crystal in nature.



There are crystal lattice defects of every dimension!

Fundamental role of defects

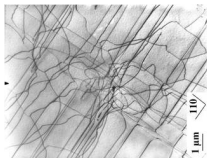
- They **influence** greatly the structural properties of metals (e.g. conductivity, malleability)
- They allow a much **wider spectrum** of mechanical properties than perfect crystals
- They can be **manipulated** to create a material with desired properties

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FOCUS ON DISLOCATIONS (LINE DEFECTS)

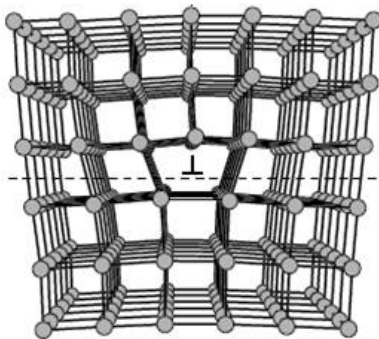
Dislocations



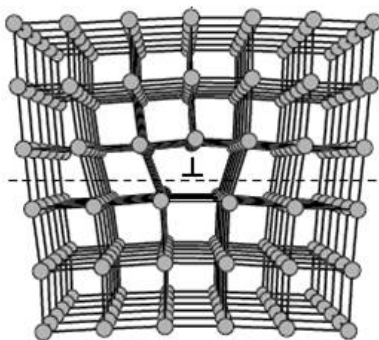
REAL DISLOCATIONS

- Curved (loops)
- Entangled

Idealised Dislocations



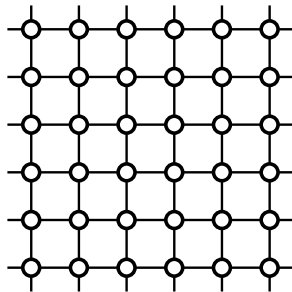
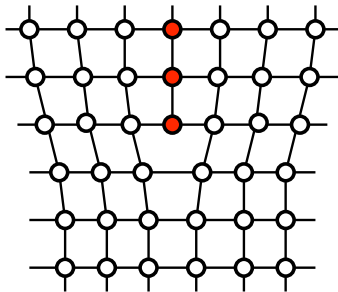
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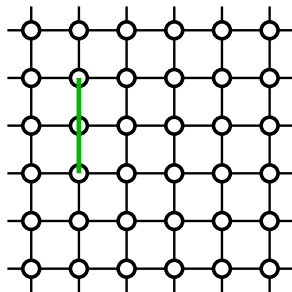
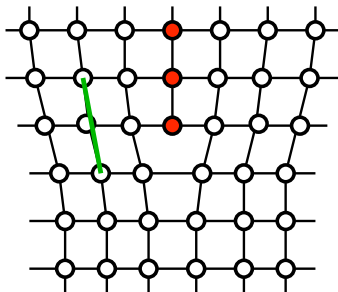
Idealised **edge** dislocation in a crystal lattice

- The direction of the dislocation line ($\xi = e_3$) is orthogonal to the Burgers vector

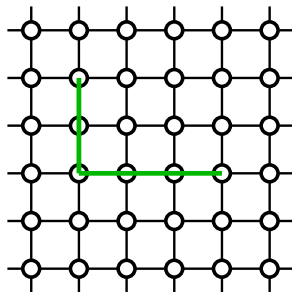
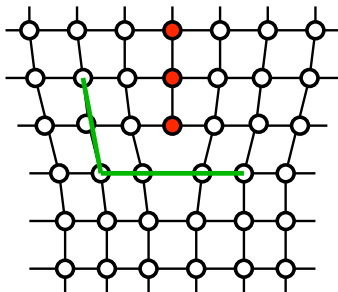
What is the Burgers vector?



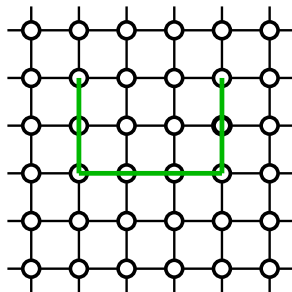
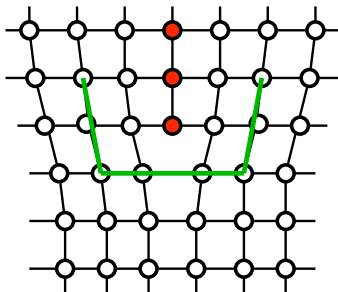
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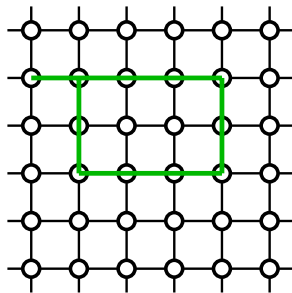
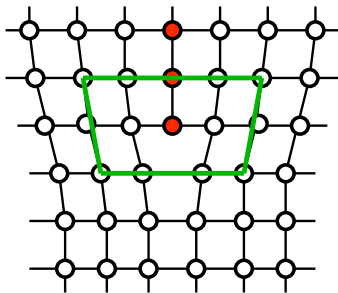
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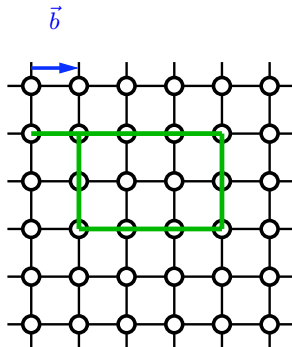
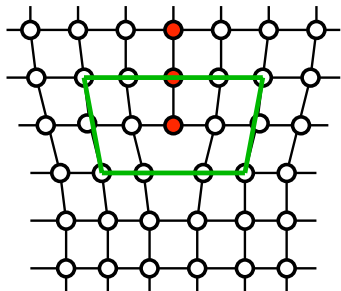
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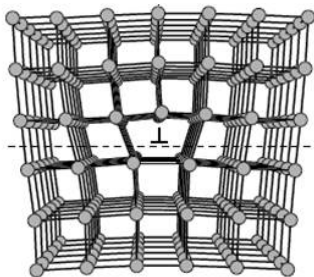


What is the Burgers vector?



The **Burgers vector** $\vec{b}$ quantifies the difference between the distorted lattice around the dislocation and the perfect lattice (vector signature of the defect)

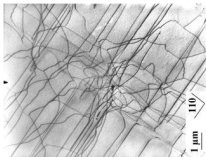
Idealised Dislocations



Idealised edge dislocation in a crystal lattice

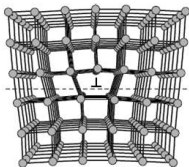
- The dislocation line ($\xi = e_3$) is orthogonal to the Burgers vector ($b = \varepsilon e_1$)
- Plane orthogonal to $b \times \xi$ (generated by b and ξ) is called the slip plane
- For **screw** dislocations ξ is parallel to b (any plane containing b is a possible glide plane) **screw like vortices in superconductors**

Dislocations



REAL DISLOCATIONS

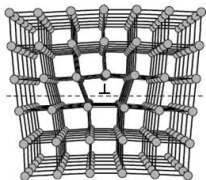
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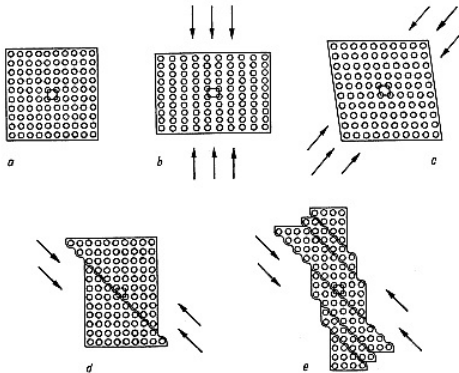
- Straight
- Parallel
- Edge

Dislocations



- Q.** Why are dislocations so important?
- A.** They make metals easier to deform.

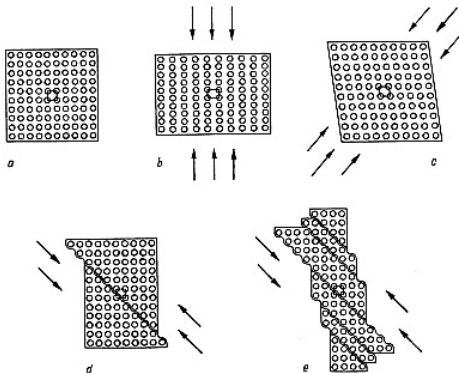
Dislocations and Plastic deformation



- Elastic: same bonds

- Plastic: new bonds

Dislocations and Plastic deformation

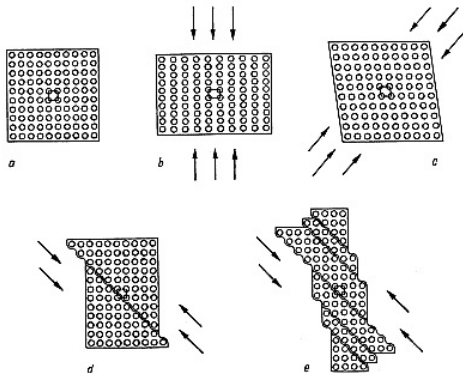


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* Plastic deformation: relative slip of atoms

Dislocations and Plastic deformation

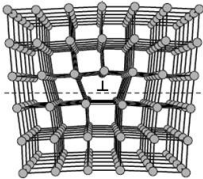


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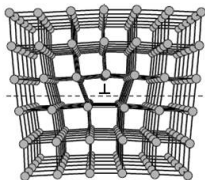
- * Plastic deformation: relative slip of atoms
- * Dislocations favour the slip, making plastic deformation easier

Dislocations



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AIM: SCALE BRIDGING

Scales in describing dislocations

continuum plasticity (mm)



dislocation densities (μm)



discrete dislocations (10 nm)



atomistic scale (0.1 nm)

Scales in describing dislocations

continuum plasticity (mm)

→ only plastic strain

dislocation densities (μm)

~> individual dislocations invisible



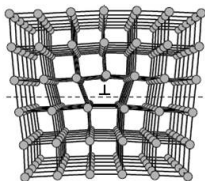
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Dislocations



Q. Why are dislocations so important?

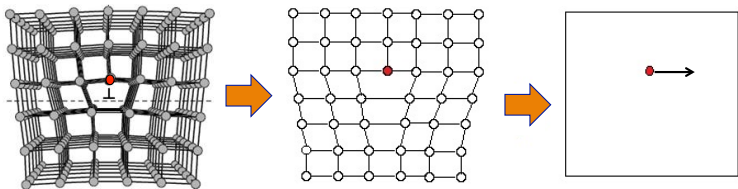
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AIM: SCALE BRIDGING

- Incorporate the presence of dislocations (well-understood at the *microscopic* scale) in a macroscopic continuum plasticity model (in terms of a *dislocation density*)
- Derive plasticity models (usually phenomenological) from dislocation models - ansatz free!
- Predict the distribution of dislocations and their dynamics

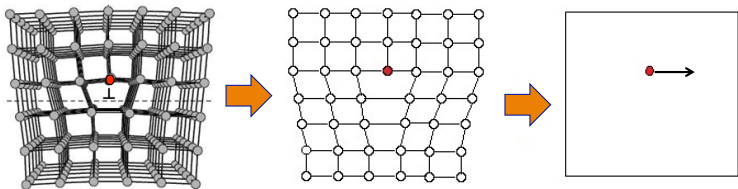
Which model?

Semi-discrete 2d dislocation model



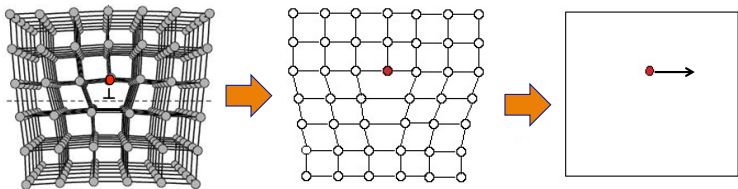
- Straight and parallel dislocation lines $\rightsquigarrow$ 2d-model

Semi-discrete 2d dislocation model



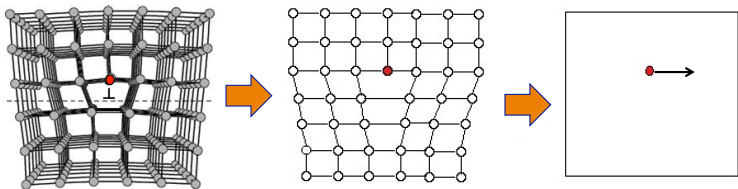
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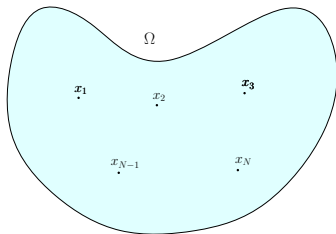
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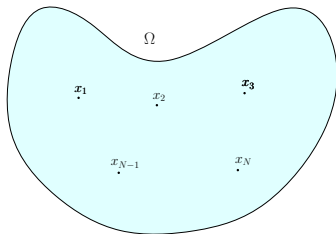
- Straight and parallel dislocation lines $\rightsquigarrow$ 2d-model
- Assume scale separation $\rightsquigarrow$ semi-discrete model
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- * Purely discrete (atomistic) dislocation models: Ortnner, Hudson, Buze, Ariza, Ortiz, Ponsiglione, De Luca, Alicandro, Garroni, etc.
- * 3d mathematical models: Garroni, Conti, Müller, Ortiz, Marziani, Scala

Semi-discrete 2d dislocation model



- * $\Omega \subset \mathbb{R}^2$ reference configuration
- * $x_1, \dots, x_n$ dislocations locations
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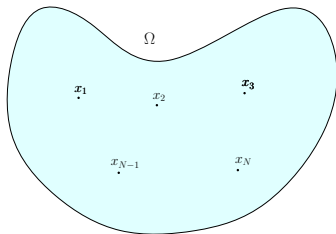
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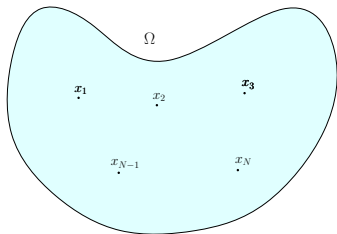
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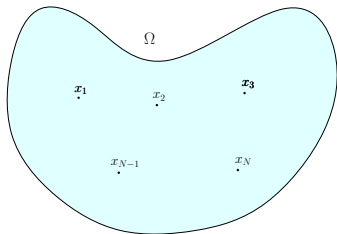
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Interpretation

$\nabla u \rightsquigarrow \beta$ (elastic strain), $D^s u \rightsquigarrow \beta_p = (-\varepsilon e_1) \otimes e_2 d\mathcal{H}^1 \llcorner \Sigma$ (plastic strain)

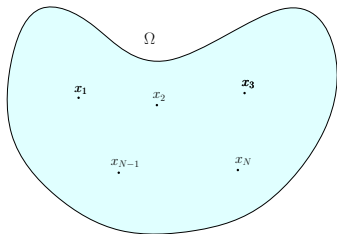
Semi-discrete 2d dislocation model



- * $\Omega \subset \mathbb{R}^2$ reference configuration
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- W ?

Linear model: $W(\beta) = \frac{1}{2}\mathcal{C}\beta : \beta$

(Conti, Müller, Garroni, Leoni, Cermelli, Ponsiglione, Alicandro, De Luca, Ortiz, Fanzon, Scala, Palombaro etc..)

$$E_n(\beta, \mu) = \frac{1}{2} \int_{\Omega} \mathcal{C}\beta : \beta \, dx, \quad \text{Curl}\beta = \mu = \frac{1}{n} \sum_{i=1}^n b_i \delta_{x_i}$$

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- In a small ball $B_r(x_0)$

$$\int_{B_r(x_0)} |\beta|^2 \, dx \sim \frac{|b|^2}{2\pi} \int_0^r \frac{1}{\rho} \, d\rho = +\infty \quad \text{☹️}$$

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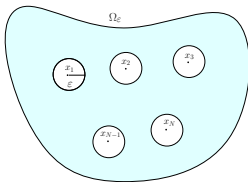
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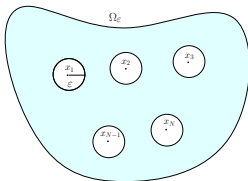
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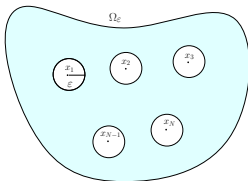
Discrete analysis for screws (Ponsiglione) $\Rightarrow$ energy in ε -cores is a factor $|\log \varepsilon|$ smaller than energy in $\Omega_{\varepsilon}(\mu)$

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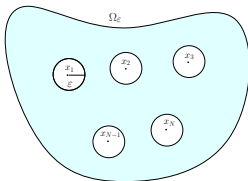
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- * **Scaling** of regularised energy?

Energy scaling: close vs far from dislocations

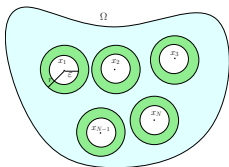
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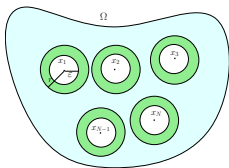
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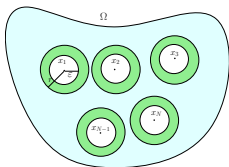
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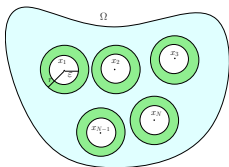
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- Write $B_r \setminus B_\varepsilon = \bigcup_{k=0}^N (B_{2^{k+1}\varepsilon} \setminus B_{2^k\varepsilon})$, $2^{N+1}\varepsilon = r \Rightarrow N \sim |\log \varepsilon|$

Energy scaling: close vs far from dislocations

Close to dislocations (self): $E_{n,\varepsilon}^{\text{self}}(\beta, \mu) \simeq \frac{1}{n} \varepsilon^2 |\log \varepsilon|$

- $E_{n,\varepsilon}$ only controls β^{sym} $\Rightarrow$ need to use Korn's inequality!

$$\begin{aligned}
 \int_{B_{2R} \setminus B_R} |\beta^{\text{sym}}|^2 dx &\stackrel{???}{\geq} C \int_{B_{2R} \setminus B_R} |\beta - A|^2 dx \\
 &= C \int_R^{2R} d\rho \int_{\partial B_\rho} |\beta - A|^2 ds \\
 &\geq C \int_R^{2R} \frac{d\rho}{2\pi\rho} \left| \int_{\partial B_\rho} (\beta - A) \tau ds \right|^2 \\
 &= C \int_R^{2R} \frac{d\rho}{2\pi\rho} \left| \int_{\partial B_\rho} \beta \tau ds \right|^2 \sim \frac{\varepsilon^2}{n^2}
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$$\Rightarrow \int_{B_r \setminus B_\varepsilon} |\beta^{\text{sym}}|^2 dx \sim |\log \varepsilon| \frac{\varepsilon^2}{n^2}$$

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- By classical Korn in $U^\pm$, there exist $A^\pm$ skw

$$\|\nabla u^\pm - A^\pm\|_{L^2(U^\pm)} \leq C \|\text{sym}(\nabla u^\pm)\|_{L^2(U^\pm)}$$

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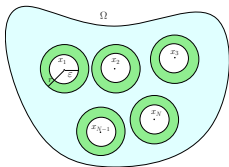
$$\Rightarrow \|\beta - A^\pm\|_{L^2(U^\pm)} \leq C \|\beta^{\text{sym}}\|_{L^2(U^\pm)}$$

- I can take $A = A^+$ or $A = A^-$ since

$$|A^+ - A^-|^2 a = \int_{U^+ \cap U^-} |A^+ - A^-|^2 dx \leq C \|\beta^{\text{sym}}\|_{L^2(U^\pm)}^2$$

Energy scaling: close vs far from dislocations

$$\begin{aligned} E_{n,\varepsilon}(\beta, \mu) &= \frac{1}{2} \int_{\Omega_\varepsilon(\mu)} \mathcal{C}\beta : \beta \, dx, \quad \text{Curl}\beta = \mu = \frac{1}{n} \sum_{i=1}^n b_i \delta_{x_i} \\ &= \underbrace{E_{n,\varepsilon}^{\text{self}}(\beta, \mu)}_{\text{"close" energy}} + \underbrace{E_{n,\varepsilon}^{\text{far}}(\beta, \mu)}_{\text{"far" energy}} \end{aligned}$$

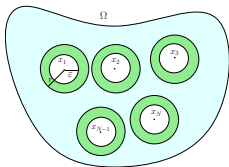


- Close to dislocations (self)

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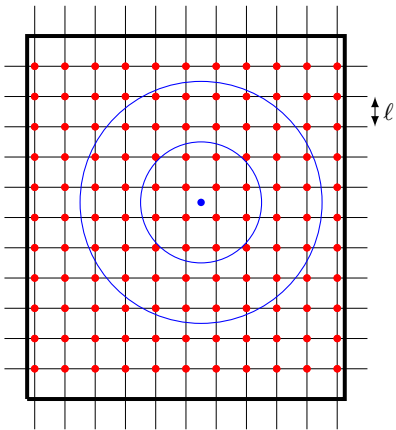
$$E_{n,\varepsilon}^{\text{self}}(\beta, \mu) \simeq \frac{1}{n} \varepsilon^2 |\log \varepsilon|$$

- Far from dislocations

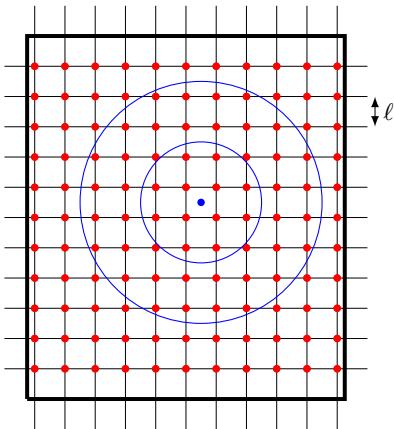
$$E_{n,\varepsilon}^{\text{far}}(\beta, \mu) \simeq \varepsilon^2$$

Energy scaling: far from dislocations

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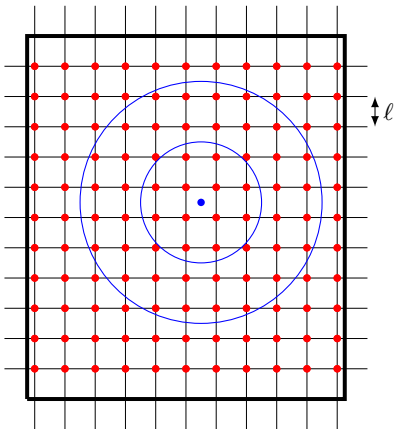


Energy scaling: far from dislocations



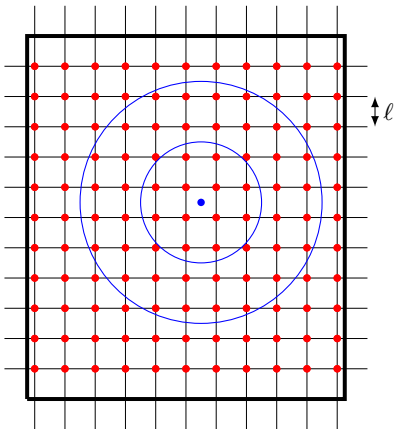
- Dislocations in uniform grid, $\ell \sim \frac{1}{\sqrt{n}}$, $x \in \Omega$

Energy scaling: far from dislocations



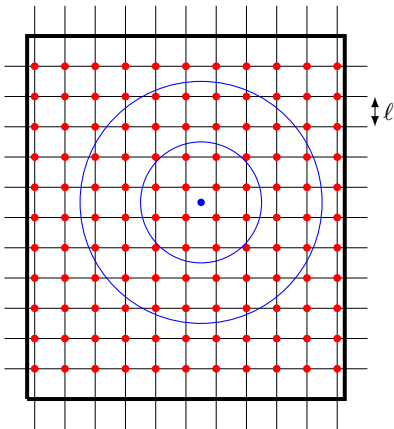
- Dislocations in uniform grid, $\ell \sim \frac{1}{\sqrt{n}}$, $x \in \Omega$
- In $B_{2r}(x) \setminus B_r(x)$ there are $\frac{r^2}{\ell^2} = nr^2$ dislocations

Energy scaling: far from dislocations



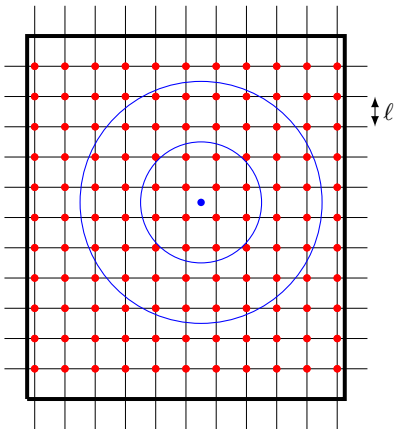
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- strain at x due to dislocations in $B_{2r}(x) \setminus B_r(x)$

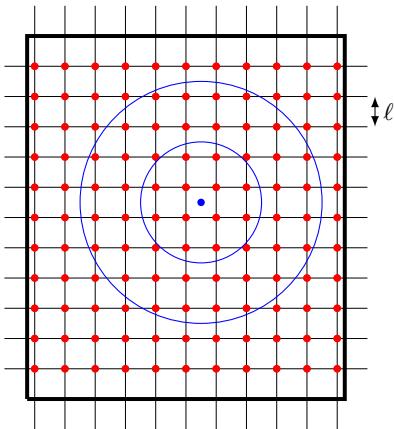
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$$|\beta(x)| \sim \sum_{i: x_i \in B_{2r}(x) \setminus B_r(x)} \underbrace{\frac{\varepsilon}{n|x-x_i|}}_{\in (r, 2r)} \sim (nr^2) \frac{\varepsilon}{nr} = \varepsilon r$$

Energy scaling: far from dislocations

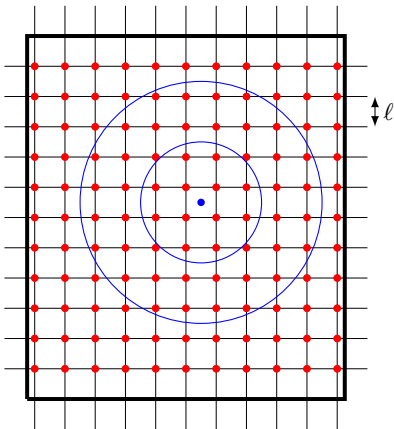


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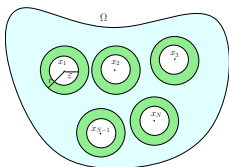
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$$|\beta(x)| \sim \sum_{k=0}^K \varepsilon r_k = \sum_{k=0}^K \varepsilon 2^k \ell \sim \varepsilon 2^K \ell \sim \varepsilon \implies \int_{\Omega} |\beta|^2 dx \sim \varepsilon^2$$

Energy scaling: close vs far from dislocations

$$\begin{aligned} E_{n,\varepsilon}(\beta, \mu) &= \frac{1}{2} \int_{\Omega_\varepsilon(\mu)} C\beta : \beta \, dx, \quad \text{Curl}\beta = \mu = \frac{1}{n} \sum_{i=1}^n b_i \delta_{x_i} \\ &= \underbrace{E_{n,\varepsilon}^{\text{self}}(\beta, \mu)}_{\text{"close" energy}} + \underbrace{E_{n,\varepsilon}^{\text{far}}(\beta, \mu)}_{\text{"far" energy}} \end{aligned}$$



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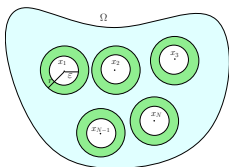
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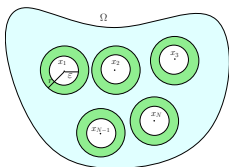
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Note: Same order if $n \sim |\log \varepsilon|!$ (critical scaling)

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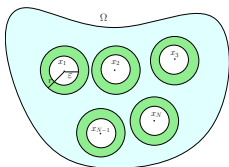
Note: We are assuming **separation** of dislocations: $\varepsilon \ll \rho_\varepsilon \ll 1$

(No separation: De Luca, Garroni, Ponsiglione, Ginster)

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Note: Nonlinear energies same scalings

(Müller, Scardia, Zeppieri, Lauteri, Luckhaus, Palombaro, Garroni, Marziani, Scala, Ginster)

Critical energy scaling

$$\tilde{E}_{n,\varepsilon}(\beta, \mu) = \frac{1}{\varepsilon^2 |\log \varepsilon|^2} \int_{\Omega_\varepsilon(\mu)} \frac{1}{2} \mathcal{C} \beta : \beta \, dx$$

$$\operatorname{Curl} \beta = 0 \quad \text{in } \Omega_\varepsilon(\mu), \quad \int_{\partial B_\varepsilon(x_i)} \beta \tau = b_i, \quad |b_i| = \varepsilon$$

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Result (Garroni-Leoni-Ponsiglione; Müller-Scardia-Zepieri; De Luca; Ginster etc.)

$$\tilde{E}_{n,\varepsilon} \longrightarrow \int_{\Omega} \frac{1}{2} \mathcal{C} \beta : \beta \, dx + \int_{\Omega} \varphi \left(\frac{d\mu}{d|\mu|} \right) d|\mu|, \quad \operatorname{Curl} \beta = \mu$$

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- Compactness by Korn inequality (Rigidity estimate)
- φ relaxation of the minimal self-energy of a single dislocation

$$\psi(b) = \lim_{\varepsilon \rightarrow 0} \frac{1}{|\log \varepsilon|} \min \left\{ \int_{B_{\rho_\varepsilon} \setminus B_\varepsilon} \frac{1}{2} \mathcal{C} \eta : \eta \, dx : \eta \in L^2(B_{\rho_\varepsilon} \setminus B_\varepsilon), \right. \\ \left. \operatorname{Curl} \eta = 0 \text{ in } B_{\rho_\varepsilon} \setminus B_\varepsilon, \int_{\partial B_\varepsilon} \eta \tau \, ds = b \right\}$$