A multi-scale analysis of dislocations in nanowire heterostructures

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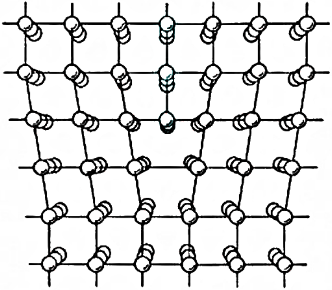
ACMAC, University of Crete, 28 March 2013

Dislocations: defects in the crystal structure of a metal



Edge dislocation in a crystal lattice

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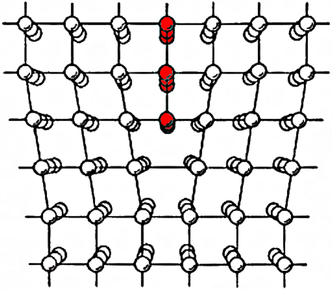
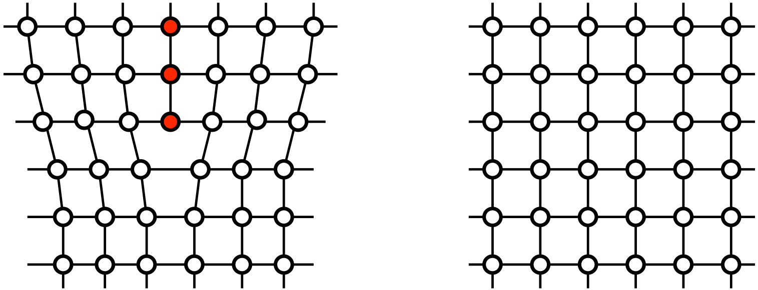


Edge dislocation in a crystal lattice

The Burgers circuit and the Burgers vector



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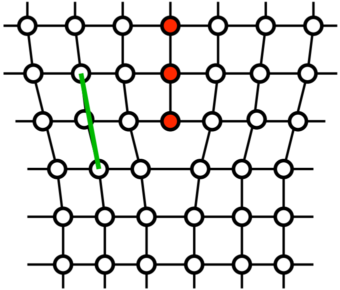

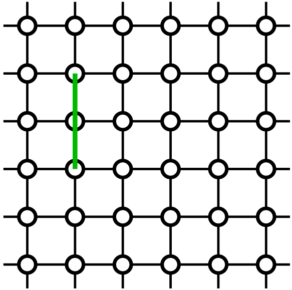

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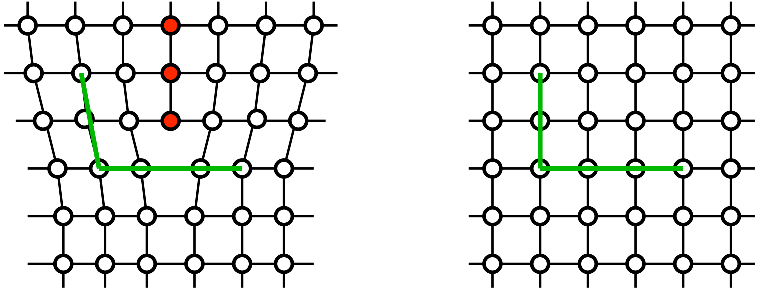

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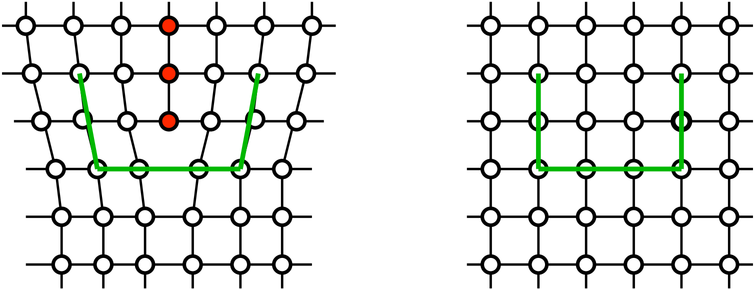

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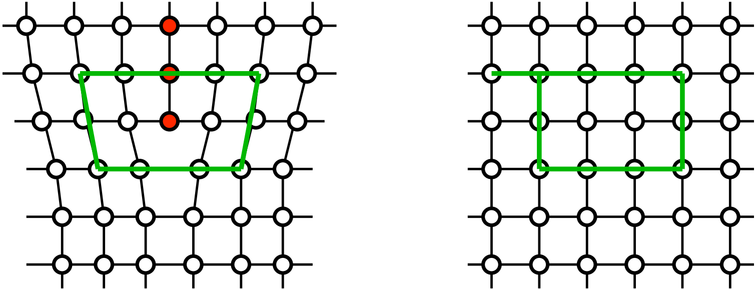

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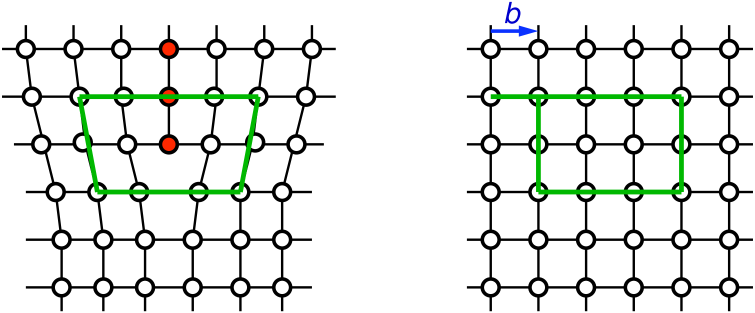
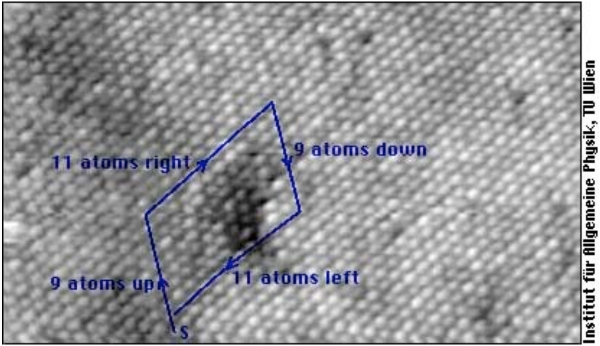
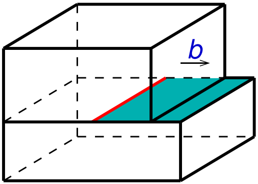


The Burgers vector b quantifies the difference between the distorted lattice around the dislocation and the perfect lattice

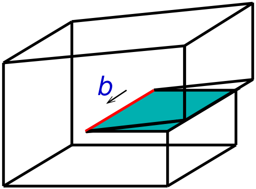

11 atoms right
9 atoms down
9 atoms up
11 atoms left
S
Institut für Allgemeine Physik, TU Wien

Continuum definition of dislocations:

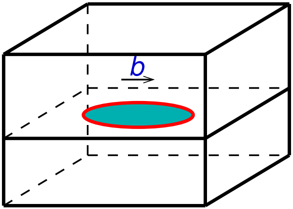
Lines on slip planes separating regions undergoing different slips (Volterra 1905)



edge dislocation



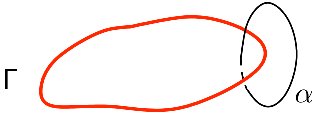
screw dislocation



dislocation loop

Look at deformations $u : \Omega \to \mathbb{R}^3$ such that

$$Du = \nabla u\, dx + b \otimes \nu\, d\mathcal{H}^2 \llcorner \mathcal{S} \quad \partial\mathcal{S} = \Gamma$$



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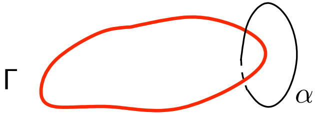


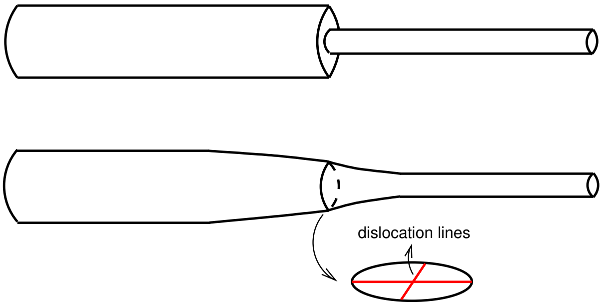
In presence of dislocations ∇u is not a gradient and

$$\mathrm{curl}(\nabla u) = -b \otimes \dot{\Gamma} \, d\mathcal{H}^1 \llcorner \Gamma$$

$$\int_\alpha \nabla u \cdot \dot{\alpha} = b \, \mathrm{link}(\alpha, \Gamma)$$

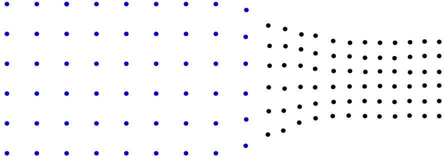
$$\Longrightarrow |\nabla u(x)| \sim \frac{1}{\mathrm{dist}(x, \Gamma)} \Longrightarrow \nabla u \notin L^p(\Omega) \text{ for } p \geq 2$$

Nanowire heterostructures: nanowires made of two or more materials featuring different lattice constants

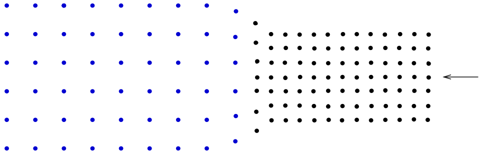


Macroscopic picture of the beam before and after interfacial bonding

Longitudinal section of the beam in the microscopic picture



elastic strain

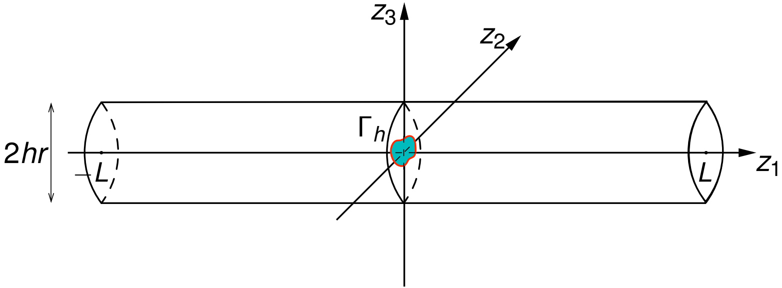


elastic strain

+

dislocation

Mathematical modeling in the continuous setting (Müller-P. 2012)



reference configuration: $\Omega_h = (-L, L) \times hD_r$ "thin" domain

dislocation line: $\Gamma_h = h\Gamma\,, \qquad \Gamma \subset D_r$

Burgers vector: $hb, \quad |b| = 1$

General strategy:

- we assume that the equilibrium configurations are minimizers of an associated elastic energy E_h
- $\min E_h$ depends on Γ $\rightsquigarrow$ show that

$$\inf_{\Gamma} \min E_h < \min E_h|_{\Gamma=\varnothing} \quad \text{for large } r$$

- replace E_h by a simpler functional that does not depend on the small parameter h and such that

$$\min E_h \to \min E$$

Tool: Γ-convergence (De Giorgi 1975)

$$E_h \xrightarrow{\Gamma} E_0$$

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- (Ansatz-free lower bound) $\forall\, u_h, u$ such that $u_h \to u$ it holds

$$E_0(u) \le E_h(u_h) + o(1) \quad \text{as} \quad h \to 0$$

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- (Existence of a "recovery sequence") $\forall\, u \;\; \exists\, \bar{u}_h$ such that $\bar{u}_h \to u$ and

$$E_h(\bar{u}_h) \to E_0(u) \quad \text{as} \;\; h \to 0$$

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Fundamental property of Γ-convergence

$$E_h \xrightarrow{\Gamma} E_0 \quad + \quad \text{“compactness”}$$

$$\Downarrow$$

$$\min\{E_h(u) \colon u \in X_h\} \quad \to \quad \min\{E_0(u) \colon u \in X_0\}$$

The elastic energy (per unit cross-section) has the form

$$\mathcal{E}_h(F) = \frac{1}{h^2} \int_{\Omega_h} W(z, F(z))\, dz$$

$$F \in L^p(\Omega_h; \mathbb{M}^{3\times 3}) \quad p \in (1,2)$$

$$\operatorname{curl} F = -hb \otimes \dot{\Gamma}_h \, d\mathcal{H}^1 \llcorner \Gamma_h$$

F is locally a gradient in $\Omega_h \setminus \Gamma_h$

Assumptions on $W : \Omega_h \to [0, +\infty)$

$$W(x, A) = \begin{cases} W_1(A) & \text{if } x_1 \in (-L, 0) \\ W_2(A) & \text{if } x_1 \in (0, L) \end{cases}$$

- $W_i \in C^0(\mathbb{M}^{3\times 3})$

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- $W_i(RF) = W_i(F) \quad \forall \; F \in \mathbb{M}^{3\times 3}, \; R \in SO(3)$ (frame-indifference)
- mixed growth conditions: $\exists \; C_1, C_2 > 0, \; 1 < p < 2$ such that $\forall \; F \in \mathbb{M}^{3\times 3}$

$$C_1 \left(\operatorname{dist}^2(A, SO(3)) \wedge (|A|^p + 1)\right) \leq W_1(F) \leq C_2 \left(\operatorname{dist}^2(A, SO(3)) \wedge (|A|^p + 1)\right)$$

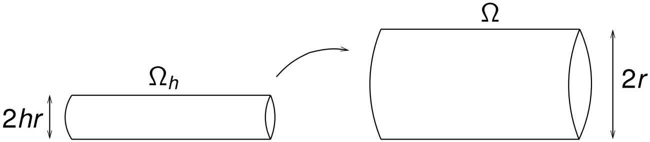
$$C_1 \left(\operatorname{dist}^2(A, SO(3)H) \wedge (|A|^p + 1)\right) \leq W_2(F) \leq C_2 \left(\operatorname{dist}^2(A, SO(3)H) \wedge (|A|^p + 1)\right)$$

$H = \operatorname{diag}(\zeta_1, \zeta_2, \zeta_3)$, H and I “incompatible”

(typical H is $H = cI$)

Rescale Ω_h to a fixed domain Ω

$$z_1 = x_1$$
$$z_2 = hx_2$$
$$z_3 = hx_3$$



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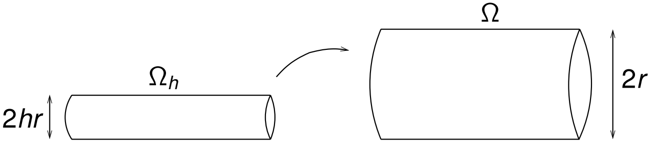

$$G(z(x)) =: F_h(x)$$

$$F_h := \left(F^1 \middle| \frac{1}{h} F^2 \middle| \frac{1}{h} F^3 \right)$$

$$\mathcal{E}^h(G) = \frac{1}{h^2} \int_{\Omega_h} W(z, G(z))\, dz = \int_{\Omega} W(x, F_h(x))\, dx =: \mathcal{I}^h(F)$$

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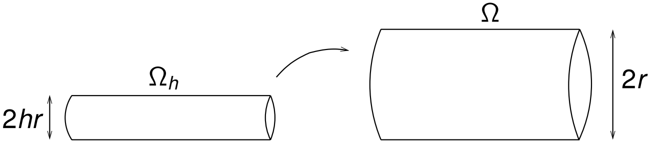

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Goal: Identify the Γ-limit $\mathcal{I}$ of the rescaled functional $\frac{1}{h}\mathcal{I}^h$ as $h \to 0$ and show that $\mathcal{I}$ favours dislocations for sufficiently large r

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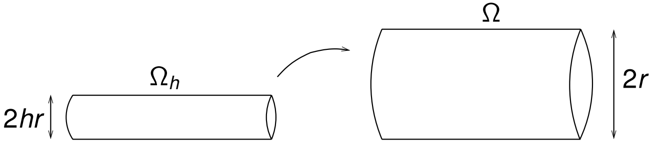

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$\Gamma - \lim \frac{1}{h}\mathcal{I}^h$ studied in Mora-Müller 2007 in the dislocation-free case

Theorem

- Compactness: $\frac{1}{h}\mathcal{I}^h(F^h) \leq C \Longrightarrow F^{(h)} \rightharpoonup F$ weakly in $L^p(\Omega, \mathbb{M}^{3\times 3})$

$$F = \left(u' \middle| \, 0 \, \middle| 0\right), \; u \in W^{1,\infty}((-L, L); \mathbb{R}^3), \; |u'| \leq \begin{cases} 1 & \text{a.e. in } (-L, 0) \\ \zeta_1 & \text{a.e. in } (0, L) \end{cases} \quad (*)$$

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$$\mathcal{I}(F) = \begin{cases} \sigma(\Gamma) & \text{if } F \text{ satisfies } (*) \\ +\infty & \text{otherwise} \end{cases}$$

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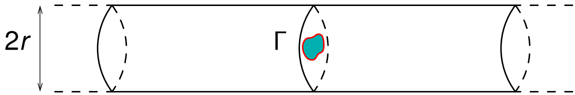
$\sigma(\Gamma)$ is the minimum cost of a transition from one well to the other

$$\sigma(\Gamma) := \inf_{M} \inf_{F} \Big\{ \mathcal{E}^\infty(F) \ :\ \mathrm{curl} F = -b \otimes \dot{\Gamma}\, d\mathcal{H}^1 \llcorner \Gamma,$$
$$F = I \text{ for } x_1 < -M, F = H \text{ for } x_1 > M \Big\}$$

$$\mathcal{E}^\infty(F) = \int_{\mathbb{R}\times D_r} W(x, F(x))\, dx$$



Key ingredient of the proof: a suitable variant of the Rigidity Estimate

Rigidity Estimate in $W^{1,2}$ (Friesecke - James - Müller)

There exists a constant $C > 0$: for every $u \in W^{1,2}(\Omega;\mathbb{R}^3)$ there exists a constant rotation $R \in SO(3)$ such that

$$\int_\Omega |\nabla u - R|^2 dx \leq C \int_\Omega \mathrm{dist}^2(\nabla u, SO(3)) dx$$

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$(2, p)$ Rigidity Estimate

There exists a constant $C > 0$: for every $u \in W^{1,p}(\Omega; \mathbb{R}^3)$ there exists a constant rotation $R \in SO(3)$ such that

$$\int_\Omega |Du - R|^2 \wedge (|Du|^p + 1)\, dx \leq C \int_\Omega \operatorname{dist}^2(Du, SO(3)) \wedge (|Du|^p + 1)\, dx$$

Recall that

$$\sigma(\Gamma, r) = \inf \mathcal{E}^\infty(F), \quad \mathcal{E}^\infty(F) = \int_{\mathbb{R}\times D_r} W(x, F(x))\, dx$$

$$\sigma(\varnothing, r) \rightsquigarrow \text{ no dislocation}$$

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$$\sigma(\varnothing, 1) > \limsup_{r\to+\infty} \inf_{\Gamma} \frac{\sigma(\Gamma, r)}{r^3}$$

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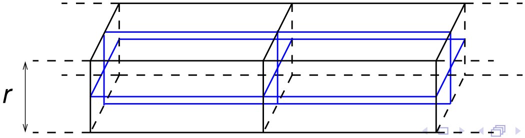
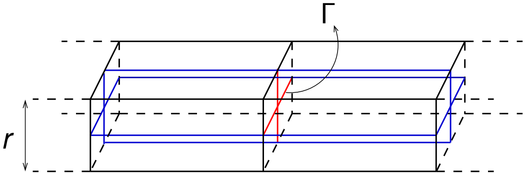
Idea of the proof

1. $\sigma(\varnothing, r) = r^3 \sigma(\varnothing, 1)$ by a simple rescaling argument
2. take u such that $\mathcal{E}^\infty(Du) = \sigma(\varnothing, r/2) + \delta$ and contruct a dislocation Γ and an ad hoc test function for $\sigma(\Gamma, r)$ by gluing together suitable translations of u defined in the four sub-cylinders



- define $\tilde{u} = u_i$ in each of the four sub-cylinder
- introduce jumps across the interface in order to match the boundary conditions
- remove the jumps across the blue planes
- let F be the “elastic” part of the gradient of such deformation



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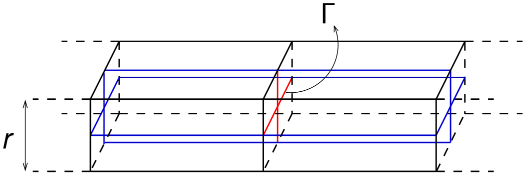

$$\sigma(\Gamma, r) \leq \mathcal{E}^\infty(F) = 4\mathcal{E}^\infty(Du) + o(r^3) = 4\sigma(\varnothing, r/2) + \delta + o(r^3)$$

$$= 4\frac{r^3}{8}\sigma(\varnothing, 1) + \delta + o(r^3)$$

A discrete model (Lazzaroni - P. - Schlömerkemper)

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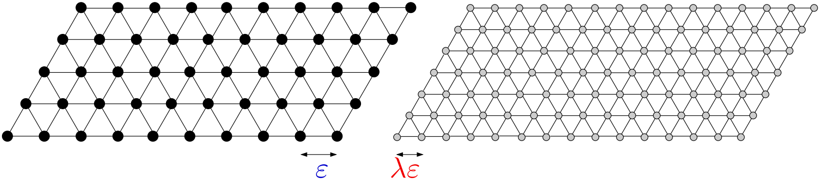
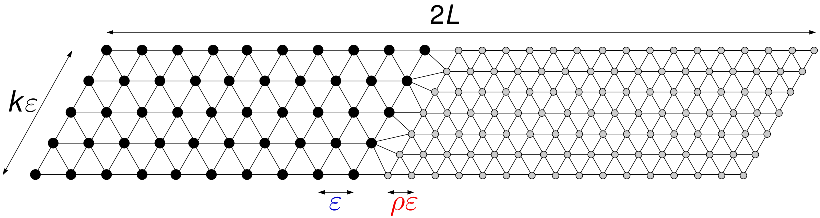
$d = 2$

Hexagonal Bravais lattices with lattice distance ε and $\lambda\varepsilon$



$$\lambda \in (0, 1)$$

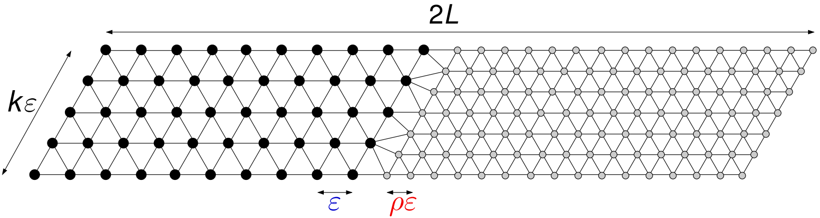
Reference configuration



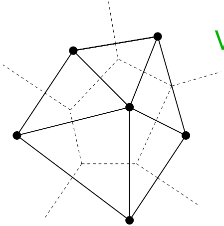
$\rho \in [\lambda, 1]$

$\rho = 1 \rightsquigarrow$ same number of lines

$\rho = \lambda \rightsquigarrow$ more lines on the right $\rightsquigarrow$ dislocations

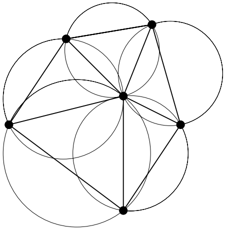


Nearest neighbors defined by the Delaunay triangulation



Voronoi diagram

Delaunay triangulation



Nearest neighbour interaction

$$\mathcal{E}_\varepsilon^{k,\rho}(u) := \frac{1}{2}\sum_{\substack{\text{NN}\\\text{left}}}\left(\left|\frac{u(x)-u(y)}{\varepsilon}\right| - 1\right)^2 + \frac{1}{2}\sum_{\substack{\text{NN}\\\text{right}}}\left(\left|\frac{u(x)-u(y)}{\varepsilon}\right| - \lambda\right)^2$$

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Remark: $\mathcal{E}_\varepsilon^{k,\rho}(u) > c > 0$ uniformly in ε because of interfacial bonds

$\Gamma - \lim_{\varepsilon\to 0} \varepsilon\,\mathcal{E}_\varepsilon^{k,1} \rightsquigarrow$ Alicandro-Braides-Cicalese (2008), B. Schmidt (2008)

Nearest neighbour interaction

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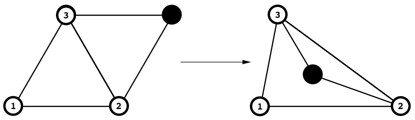
Remark: $\mathcal{E}_\varepsilon^{k,\rho}(u) > c > 0$ uniformly in ε because of interfacial bonds

Admissible deformations: $\det Du > 0$ (u identified with its piece-wise affine interpolation)

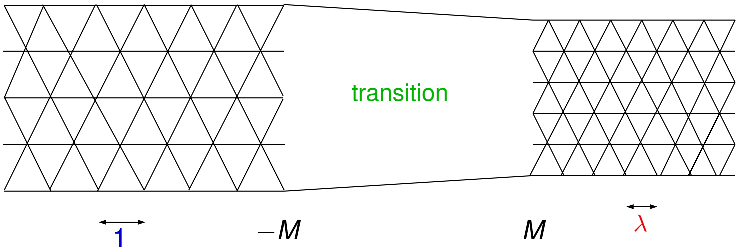


self interpenetration not allowed

Theorem. The minimal energetic cost needed to compensate the lattice mismatch is

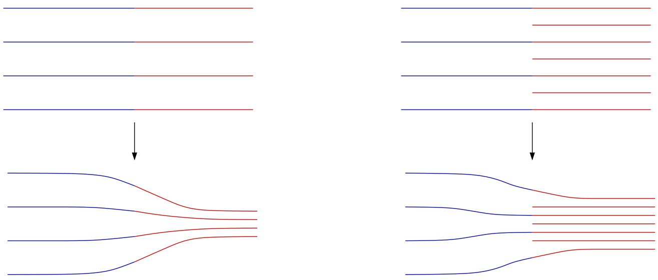
$$\sigma^d(k,\rho) := \inf_{v,M}\left\{ \mathcal{E}_1^{k,\rho}(v) : \det \nabla v > 0,\ \nabla v = I \text{ in } (-\infty,-M),\ \nabla v = \frac{\lambda}{\rho} I \text{ in } (M,+\infty) \right\}$$

$$\mathcal{E}_1^{k,\rho}(v) := \frac{1}{2}\sum_{\substack{\text{NN}\\ \text{left}}} \Big(|v(x)-v(y)| - 1\Big)^2 + \frac{1}{2}\sum_{\substack{\text{NN}\\ \text{right}}} \Big(|v(x)-v(y)| - \lambda\Big)^2$$



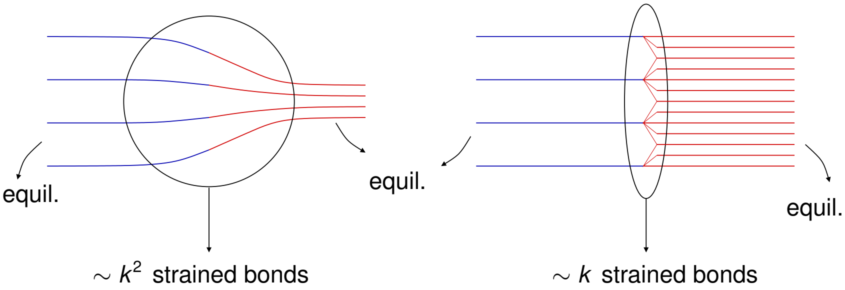
We compare two types of configurations:

defect-free dislocated



Which one is energetically more favorable when k grows?
(k = number of lines)

Theorem. $\sigma^d(k, \rho = 1) > \sigma^d(k, \rho = \lambda)$ as $k \to \infty$



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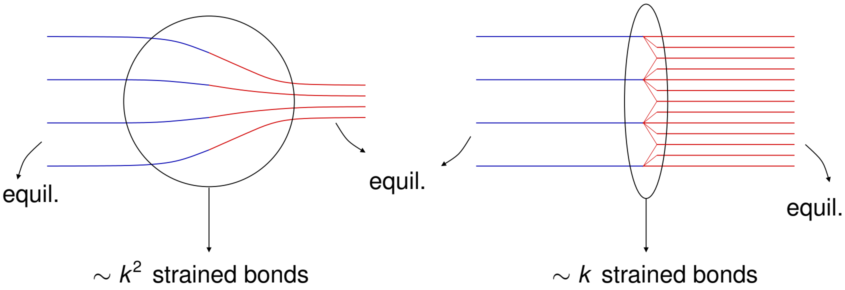
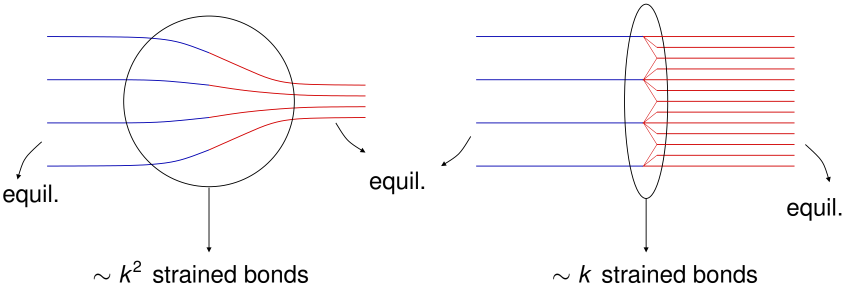


Defect-free:

rescaling argument + non-int. $\Longrightarrow$ $C_1 k^2 \leq \sigma^d(k, \rho = 1) \leq C_2 k^2$

Theorem. $\sigma^d(k, \rho = 1) > \sigma^d(k, \rho = \lambda)$ as $k \to \infty$



Defect-free:

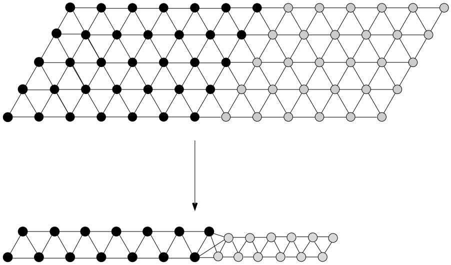
rescaling argument + non-int. $\Longrightarrow$ $C_1 k^2 \leq \sigma^d(k, \rho = 1) \leq C_2 k^2$

Dislocated:

test with the identical deformation $\Longrightarrow$ $C_3 k \leq \sigma^d(k, \rho = \lambda) \leq C_4 k$

Remark: the theorem does not hold if we remove the non-interpenetration condition $\det \nabla u > 0$

Counterexample:

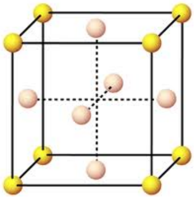


$\sigma^d(k, \rho = 1) = Ck$

linear growth

$\det \nabla u > 0 \Longrightarrow$ rigidity estimate $\Longrightarrow$ quadratic growth of $\sigma^d(k, \rho = 1)$

$d = 3$



Face Centered Cubic

Questions:

- Can we remove the non-interpenetration assumption by adding next-nearest-neighbor interactions?
- Extension of the results to the case of more general energies