Dislocations in nanowire heterostructures: from discrete to continuum

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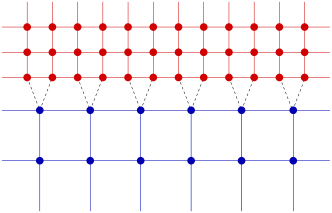
Joint work with M. Palombaro and A. Schlömerkemper

Epitaxial growth



A heterostructure is a material obtained through epitaxial growth, i.e., by deposition of atoms of one material (overlayer) on top of another material (underlayer).

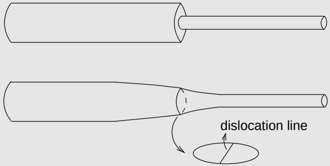
The materials have different lattice constants.

$\begin{cases} \text{Fewer atoms} & \rightarrow \text{Strain compensates the lattice mismatch} \\ \text{More atoms} & \rightarrow \text{Formation of misfit dislocations at the interface} \end{cases}$

We study the formation of dislocations in heteronanowires,
i.e., longitudinally heterostructured very thin string-shaped devices.

Aim of the work

We look for conditions for the formation of dislocations in heteronanowires.



Schematic of heteronanowire before and after interfacial bonding

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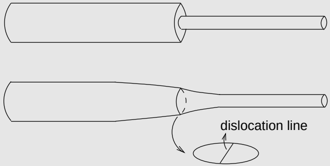


Schematic of heteronanowire before and after interfacial bonding

Our model:

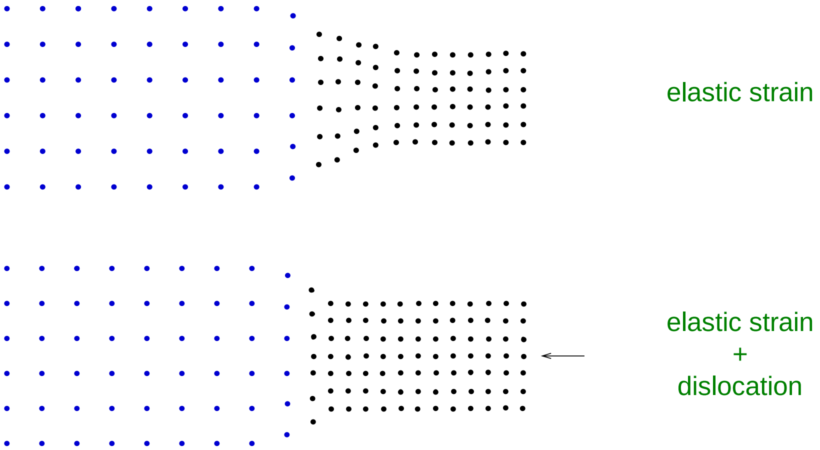
- Start from a discrete thin lattice of atoms
- Passage from discrete to continuum
- Dimension reduction $2d \longrightarrow 1d$ or $3d \longrightarrow 1d$
  In this talk: $2d \longrightarrow 1d$

Continuum model: Müller-Palombaro (2012)

Concept of the model

We compare two models, with different reference configurations.

Assumption: The system chooses the best geometry of nearest neighbours.



Figures: Longitudinal section of the beam in the microscopic picture

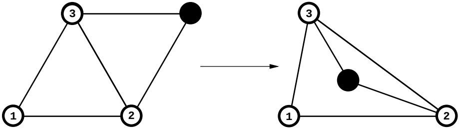
Rigidity

Our proof relies on a rigidity estimate. In order to enforce rigidity, we

- choose a rigid lattice (e.g., triangular in dim two, fcc in dim three),
- assume that the deformation satisfies the non-interpenetration.

Non-interpenetration condition

A discrete deformation u satisfies the non-interpenetration if the image of each element of the triangulation has positive orientation.
Equivalently: The Jacobian determinant of the affine interpolation is positive.



This deformation is ruled out by the non-interpenetration condition.

See e.g. Friesecke-Theil (2002), Braides-Solci-Vitali (2007), Braides-Gelli (2013)

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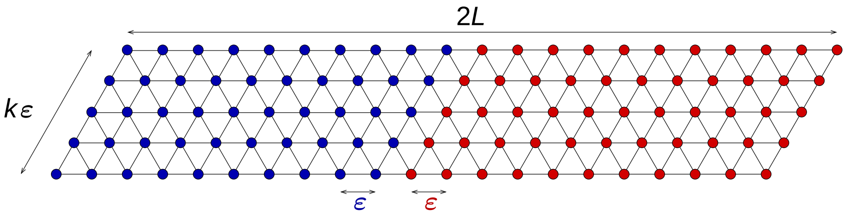
This allows us to employ the

Rigidity estimate (Friesecke-James-Müller 2002)

$$\exists C: \quad \forall u \in H^1 \; \exists R \in SO(n): \quad \|\nabla u - R\|_{L^2} \leq C \|\mathrm{dist}(\nabla u, SO(n))\|_{L^2}$$

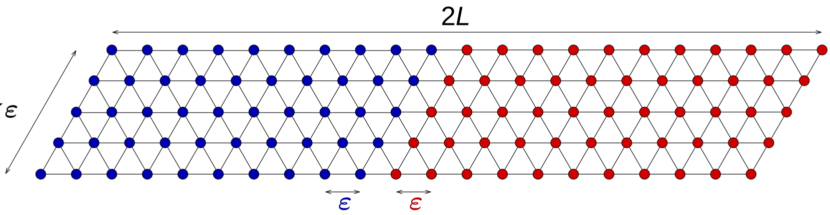
Defect-free model



Reference configuration: planar hexagonal Bravais lattice
with lattice distance $\varepsilon \to 0$.
The reference domain is a parallelogram
with length $2L$ independent of ε,
containing $k+1$ lines of atoms
$\to$ dimension reduction

Deformed configuration: equilibrium distances ε (left), $\lambda\varepsilon$ (right), $\lambda \in (0,1)$
u_ε deformation (piecewise affine interpolation)

Defect-free model

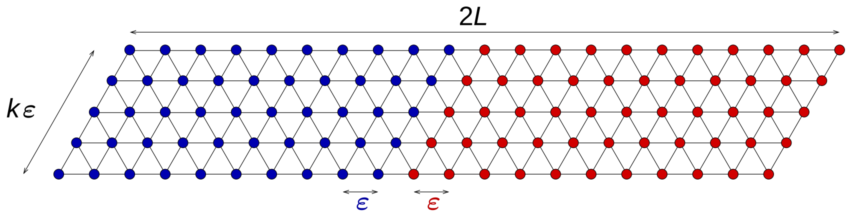


Nearest neighbours interaction

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

$\mathcal{E}_\varepsilon^{\text{df}}$ is studied in Alicandro-Braides-Cicalese (2008) and Schmidt (2008).
However, at this scaling one cannot see dislocations since $\inf \mathcal{E}_\varepsilon^{\text{df}} = O(\varepsilon)$.
Hence we rescale the functional.

Defect-free model



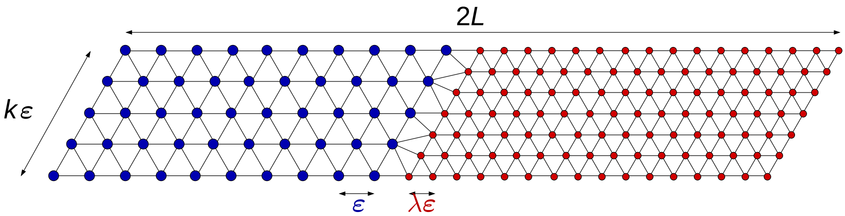
$$\mathcal{E}^{\mathrm{df}}_\varepsilon(u_\varepsilon) := \frac{\varepsilon}{2} \sum_{\substack{x \text{ left} \\ y \text{ NN}}} \left(\left| \frac{u_\varepsilon(x) - u_\varepsilon(y)}{\varepsilon} \right| - 1 \right)^2 + \frac{\varepsilon}{2} \sum_{\substack{x \text{ right} \\ y \text{ NN}}} \left(\left|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

Rescaled functional

$$\mathcal{F}^{\mathrm{df}}_\varepsilon(u_\varepsilon) := \begin{cases} \varepsilon^{-1}\, \mathcal{E}^{\mathrm{df}}_\varepsilon(u_\varepsilon) & \text{if } u_\varepsilon \text{ satisfies the non-interpenetration} \\ +\infty & \text{otherwise} \end{cases}$$

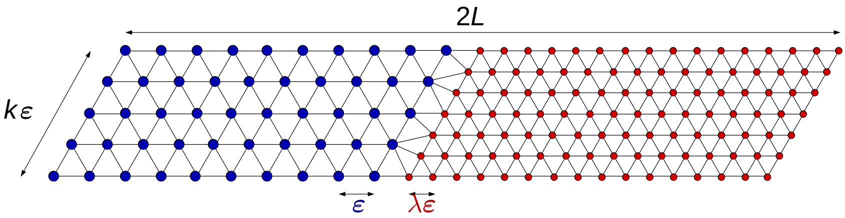
Continuum models: Mora-Müller (2007) and Müller-Palombaro (2012).

Model with dislocations

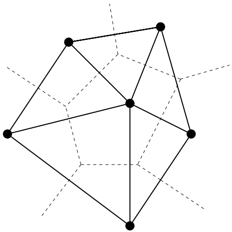


We insert more lines in the right part $\rightarrow$ Edge dislocations on the interface.
"Dislocation" means here that the coordination number is not constant
(it is the number of nearest neighbours of an internal atom).

Model with dislocations

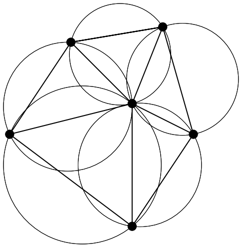


We insert more lines in the right part $\rightarrow$ Edge dislocations on the interface.
The nearest neighbours are determined by the Delaunay triangulation.



Voronoi diagram

Delaunay triangulation



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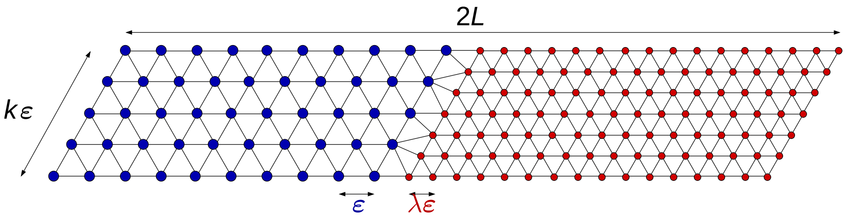
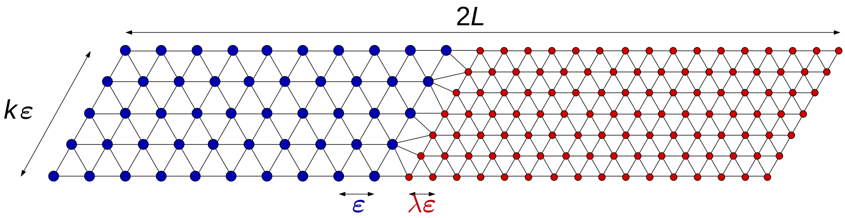


We insert more lines in the right part $\rightarrow$ Edge dislocations on the interface.
The nearest neighbours are determined by the Delaunay triangulation.

Actually it is enough to choose any triangulation with properties of uniformity:

- bounded number of nearest neighbours per atom (uniformly in k and ε)
- bounded length of the bonds in the reference (uniformly in k, linear in ε)

Model with dislocations



Nearest neighbours interaction and rescaling

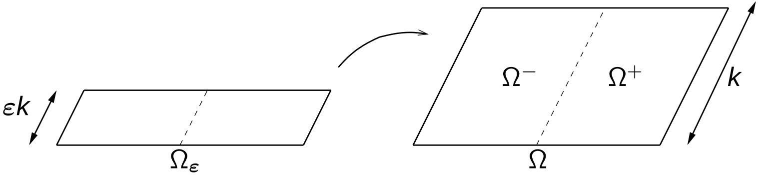
$$\mathcal{E}_\varepsilon^{\mathrm{disl}}(u_\varepsilon) := \frac{\varepsilon}{2} \sum_{\substack{x \text{ left} \\ y \text{ NN}}} \left(\left| \frac{u_\varepsilon(x) - u_\varepsilon(y)}{\varepsilon} \right| - 1 \right)^2 + \frac{\varepsilon}{2} \sum_{\substack{x \text{ right} \\ y \text{ NN}}} \left(\left|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

$$\mathcal{F}_\varepsilon^{\mathrm{disl}}(u_\varepsilon) := \begin{cases} \varepsilon^{-1} \mathcal{E}_\varepsilon^{\mathrm{disl}}(u_\varepsilon) & \text{if } u_\varepsilon \text{ satisfies the non-interpenetration} \\ +\infty & \text{otherwise} \end{cases}$$

Passage to the limit as $\varepsilon \to 0^+$

In the next slides we consider the lattice with dislocations
(similar results hold for the defect-free one).

1. Compactness: We rescale to a parallelogram independent of ε and find that (rescaled) deformations with equibounded energy converge to “short maps” $\{u \text{ depending only on } x_1\,,\ |\partial_1 u| \le 1\}$.



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2. Γ-lim inf: After passing to a dilated lattice, we bound the functional by the minimum cost of transitions between equilibria.

$$\gamma^{\mathrm{disl}}(k) = \inf_{v,M} \left\{ \mathcal{F}_1^{\mathrm{disl}}(v) \colon \nabla v = I \text{ in } (-\infty, -M), \nabla v = R \text{ in } (M, +\infty) \right\}$$

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2. Γ-lim inf: After passing to a dilated lattice, we bound the functional by the minimum cost of transitions between equilibria.

3. Γ-lim sup: That minimum cost is the Γ-limit. This is based on constructing transitions between equilibria.

Rescaling of the domain

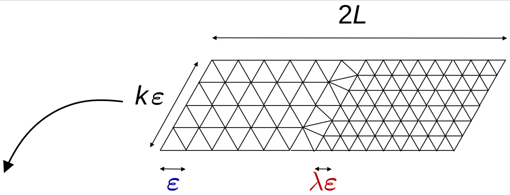
Assume $\mathcal{F}_{\varepsilon}^{\text{disl}}(u_{\varepsilon}) \leq C$.

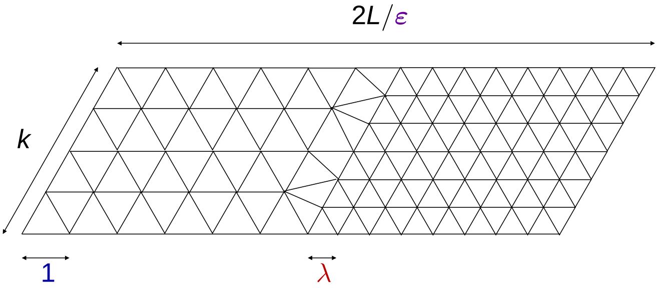
We rescale the domain

to a lattice with spacing

independent of ε,

setting $v_{\varepsilon}(x) := \varepsilon^{-1} u_{\varepsilon}(\varepsilon x)$

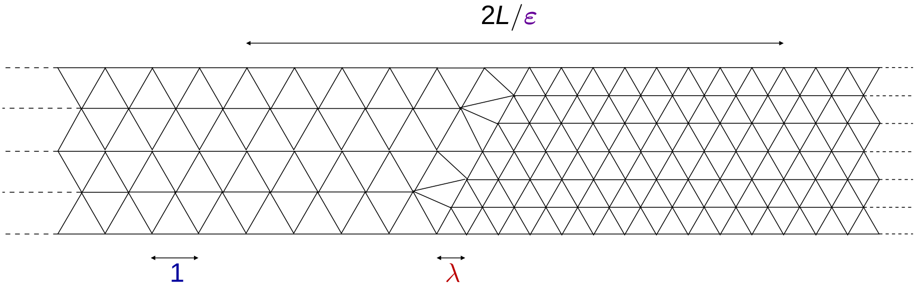




Rescaling of the domain

Next we extend the rescaled domain to an infinite strip.

We extend the deformation v_ε to $\bar{v}_\varepsilon$ defined on the infinite strip



$$\mathcal{F}^{\mathrm{disl}}_{1,\infty}(\bar{v}_\varepsilon) := \frac{1}{2}\sum_{\text{left}}\Big(\big|\bar{v}_\varepsilon(x)-\bar{v}_\varepsilon(y)\big|-1\Big)^2+\frac{1}{2}\sum_{\text{right}}\Big(\big|\bar{v}_\varepsilon(x)-\bar{v}_\varepsilon(y)\big|-\lambda\Big)^2$$

Rescaling of the domain

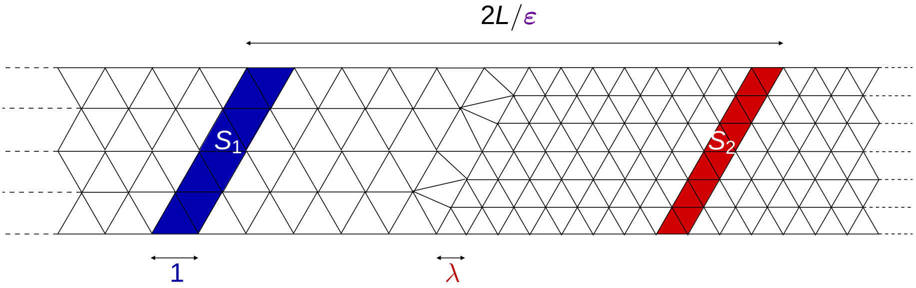
Next we extend the rescaled domain to an infinite strip.

We extend the deformation v_ε to $\bar{v}_\varepsilon$ defined on the infinite strip in this way:

Employing the rigidity estimate we find two regions S_1 and S_2 such that

$$\nabla v_\varepsilon \sim I \text{ in } S_1 \quad \text{and} \quad \nabla v_\varepsilon \sim R \in SO(2) \text{ in } S_2 .$$

Finally, $\bar{v}_\varepsilon := I$ on the left, $\bar{v}_\varepsilon := v_\varepsilon + c_1$ in between, $\bar{v}_\varepsilon := R + c_2$ on the right.



Thanks to the rigidity estimate, $\mathcal{F}^{\text{disl}}_{1,\infty}(\bar{v}_\varepsilon) \lesssim \mathcal{F}^{\text{disl}}_\varepsilon(u_\varepsilon)$.

Limit functional

We have reduced to deformations in equilibrium far from the interface:

$$\nabla v = I \text{ in } (-\infty, -M)\,, \; \nabla v = R \text{ in } (M, +\infty)$$

Limit functional

So we consider the minimum cost of transitions between equilibria:

$$\gamma^{\mathrm{disl}}(k) := \inf_{v,M} \left\{ \mathcal{F}^{\mathrm{disl}}_{1,\infty}(v) \colon \ \nabla v = I \text{ in } (-\infty, -M)\,,\ \nabla v = R \text{ in } (M, +\infty) \right\}$$

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$$\gamma^{\text{df}}(k) := \inf_{v,M} \left\{ \mathcal{F}^{\text{df}}_{1,\infty}(v) \colon \; \nabla v = I \;\text{ in } (-\infty, -M)\,, \nabla v = \lambda R \;\text{ in } (M, +\infty) \right\}$$

They are independent of R!

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Γ-convergence result (L.-Palombaro-Schlömerkemper, Comm. Math. Sci. 201?)

The (rescaled versions of the) functionals $\mathcal{F}^{\mathrm{disl}}_{\varepsilon}$, $\mathcal{F}^{\mathrm{df}}_{\varepsilon}$ Γ-converge w*-$W^{1,\infty}$ to functionals of $u \colon [-L,L] \to \mathbb{R}^2$ (reduction to 1d):

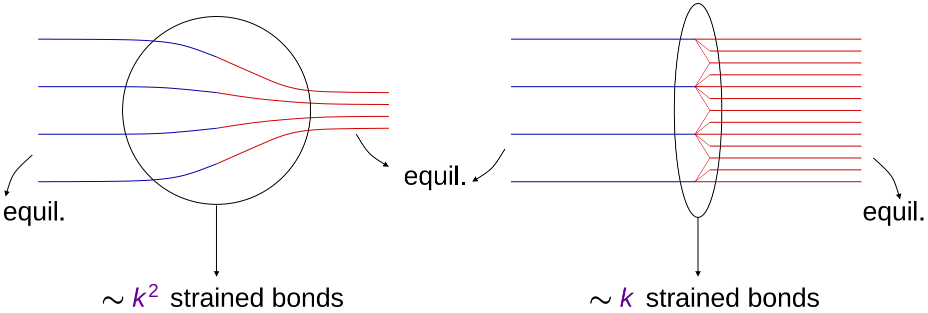
$$\mathcal{F}^{\mathrm{disl}}(u) = \begin{cases} \gamma^{\mathrm{disl}}(k) & \text{if } |\partial_1 u| \le 1 \\ +\infty & \text{otherwise} \end{cases}$$

$$\mathcal{F}^{\mathrm{df}}(u) = \begin{cases} \gamma^{\mathrm{df}}(k) & \text{if } |\partial_1 u| \le 1 \text{ (on the left) and } |\partial_1 u| \le \lambda \text{ (on the right)} \\ +\infty & \text{otherwise} \end{cases}$$

Comparison between defect-free and dislocations

Now we let the number of lines grow on both sides ($k \gg 1$).

We study the growth of γ^{df} and γ^{disl} in dependence on the number of lines:



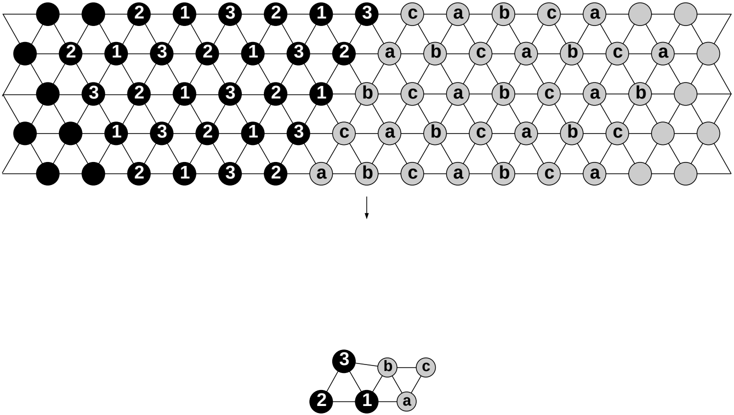
Defect-free: rescaling argument + rigidity $\Longrightarrow$ $C_1 k^2 \leq \gamma^{\mathrm{df}}(k) \leq C_2 k^2$

Dislocations: comparing with the identical deformation, $\gamma^{\mathrm{disl}}(k) \leq Ck$

This proves that dislocations are favoured for sufficiently large thickness.

The role of non-interpenetration

A deformation that violates the non-interpenetration condition:



For such a deformation the total interaction energy grows linearly in k even if the lattice is defect-free!

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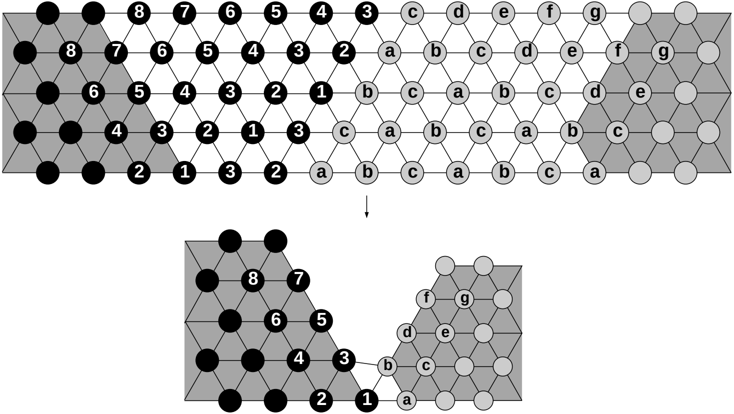

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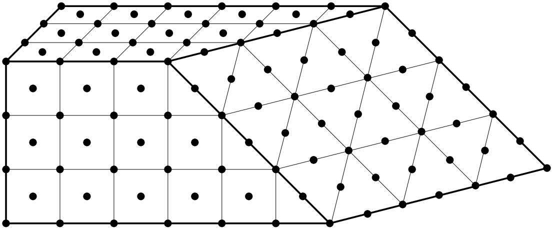
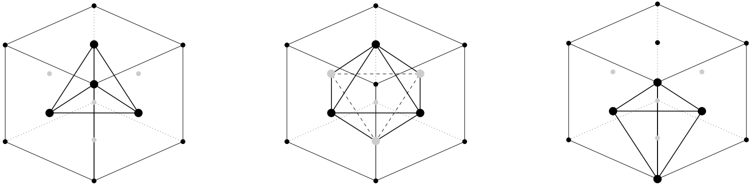
Three-dimensional model



Face-centred cubic lattice



Unit cell and tessellation

Conclusion

- We study a nanowire made of two phases, via dimension reduction and passage from discrete to continuum.
- Nearest-neighbour interactions with non-interpenetration constraint.
- By Γ-convergence we characterize the minimal energy needed to compensate the lattice mismatch.
- We compare a defect-free lattice and a lattice with dislocations.
- The cost of the defect-free model is quadratic w. r. to the number of lines, while the cost of the model with dislocations is linear.
- This shows that dislocations are favoured if the thickness is large enough.