Stability of screw dislocations in an anti-plane lattice model

Tom Hudson (Oxford)
Christoph Ortner (Warwick)

Instituto Superior Técnico, Lisboa

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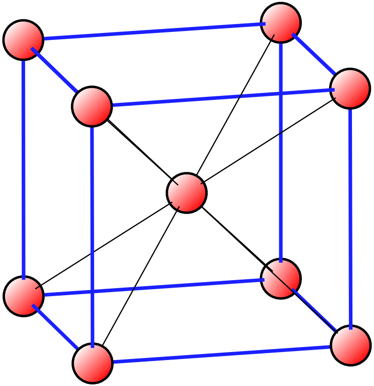
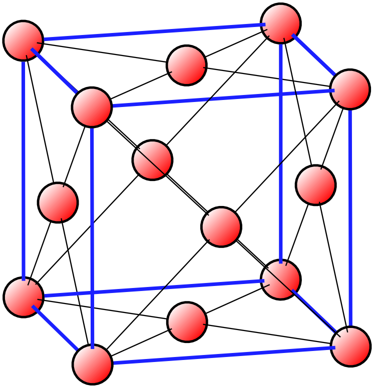
Crystalline Solids

- Many everyday solids are crystalline
- Simplest structures are Bravais lattices = affine transformations of $\mathbb{Z}^n$



Body-Centred Cubic (BCC)

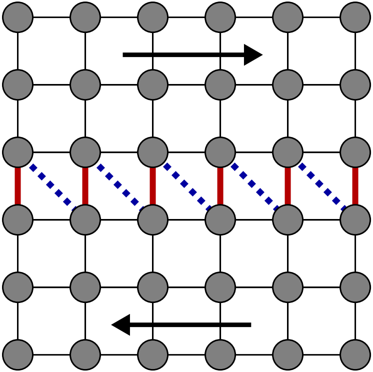


Face-Centred Cubic (FCC)

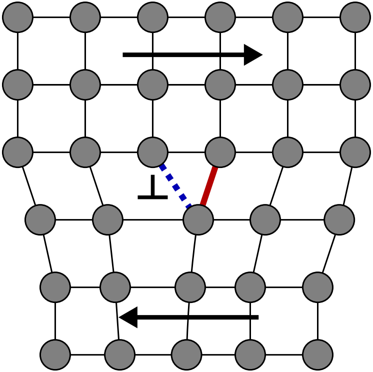
Basic Crystal Plasticity

Crystal Plasticity = **'slip'** of crystallographic planes.

Volterra (1905), Orowan (1934), Polanyi (1934), Taylor (1934):



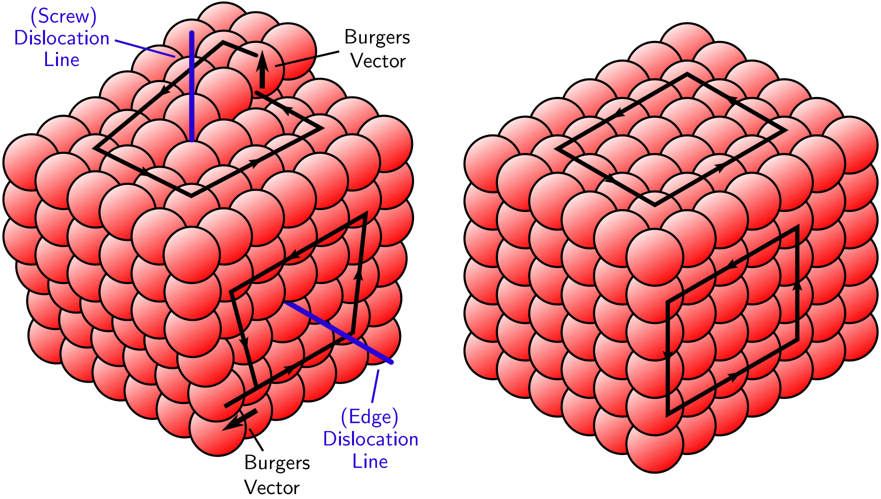
Energy required ∼ **Area**



Energy required ∼ **Length**

The Microscopic Mechanism: Dislocations

- Geometric lattice defects
- Assign them a Burgers vector, **b**, and line direction, **l**.
- Simplest types are screw (with $\mathbf{b} \parallel \mathbf{l}$) and edge (with $\mathbf{b} \perp \mathbf{l}$).



Literature Review

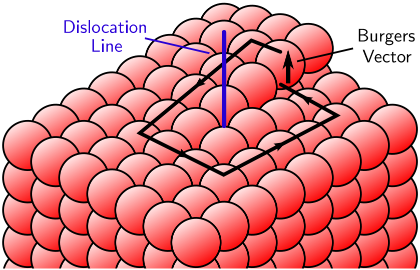
- Semi-discrete models:
  - Cermelli-Leoni (2005), Ponsiglione (2007), Scardia-Zeppieri (2012), Garroni et al (2010), De Luca et al (2012)
  - Monneau et al (2006,2008,2009,...), Blass-Morandotti (2014)
- Γ-limits of phase field models:
  - Koslowski et al (2002), Garroni et al (2005, 2006, 2011),
- Discrete (atomistic) models:
  - Ariza-Ortiz (2005): description of discrete crystal elasticity and dislocations, algebraic topology framework
  - Ponsiglione (2007): energy asymptotics of screw dislocations under anti-plane deformation
  - Alicandro-Garroni-De Luca-Ponsiglione (2013): asymptotics for energy and gradient flow dynamics of dislocations under anti-plane deformation
  - Related work: Alicandro et al (2009, 2011)

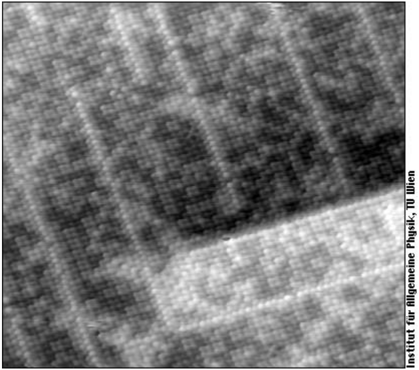
Work on dislocation statics is primarily concerned with energy asymptotics.

THIS TALK: existence of equilibrium configurations and their properties

Our Focus: Screw Dislocations

- Topological line defects
- Loosely, a 'spiral staircase' or 'vortex' in the lattice
- Burgers vector parallel to dislocation line

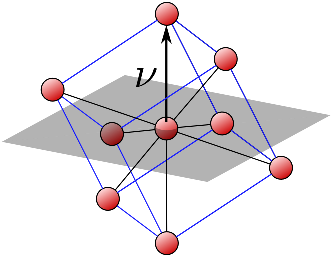




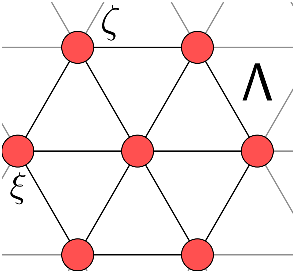
http://www.iap.tuwien.ac.at/www/surface/stm_gallery/dislocations

Setup: Anti-plane displacements

1. BCC Lattice, $\mathcal{L} := \mathrm{B}\mathbb{Z}^3$



2. Project along ν: $\Lambda = \Pi\mathcal{L} - x^0$

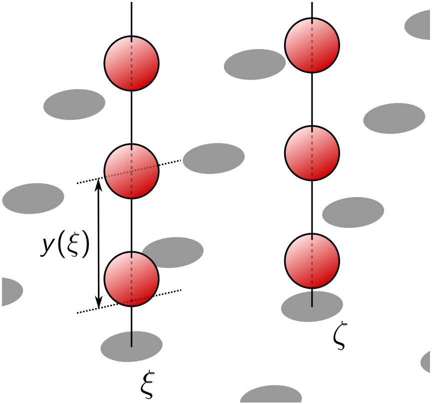


3. General deformation: $Y : \mathcal{L} \to \mathbb{R}^3$

4. Anti-plane deformation:

$$Y(x) = x + y(\Pi x - x^0)\nu,$$

where $y : \Lambda \to \mathbb{R}$



Setup: Elastic and Plastic Strain

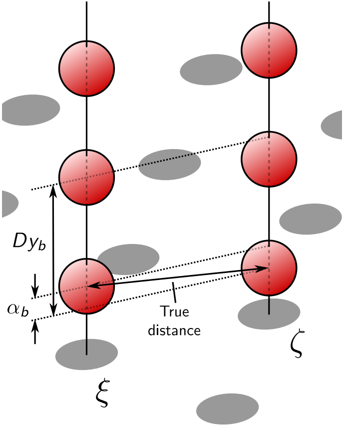
Assumption: nearest-neighbour pair interaction between columns.

$$\mathcal{B} := \{ b = (\xi, \zeta) \in \Lambda \times \Lambda \,\big|\, |\xi - \eta| = 1 \}$$

Total strain: $Dy_b := y(\xi) - y(\zeta)$

Shortest distance between atoms in 2 columns:

$$\min_{z \in \mathbb{Z}} \sqrt{1 + |Dy_b - z|^2} = \sqrt{1 + \min_z |Dy_b - z|^2} =: \sqrt{1 + |\alpha_b|^2}$$



Energy stored in a bond (between columns):

$$\psi(Dy_b) := \sum_{n \in \mathbb{Z}} \phi\Big(\sqrt{1 + |Dy_b + n|^2} \Big) = \psi(\alpha_b)$$

Elastic strain: $\alpha_b \in [-1/2, 1/2]$ **Plastic strain:** $z_b = Dy_b - \alpha_b \in \mathbb{Z}$

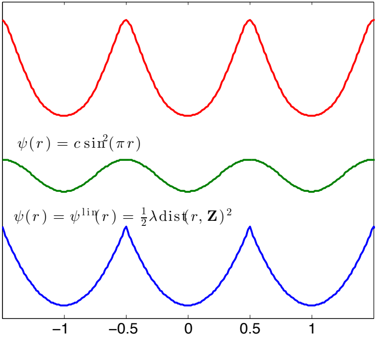
In general, these are **NOT** finite differences.

Setup: Energy Difference Functional

Energy difference functional:

$$E(y;\hat{y}) := \sum_{b\in\mathcal{B}} \Big(\psi(Dy_b) - \psi(D\hat{y}_b)\Big)$$

- Compares energy of anti-plane deformations
- Invariant under natural symmetries, e.g. translation, rotation and vertical shifts

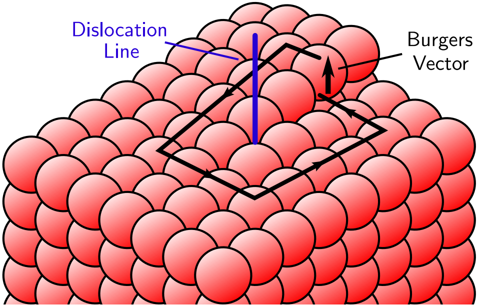


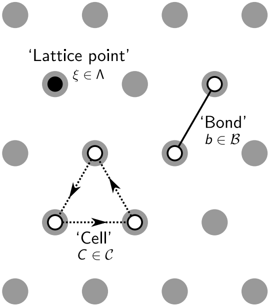
Definition: y is a globally stable equilibrium if $E(y+u;y) \ge 0$ for all $u : \Lambda \to \mathbb{R}$ with compact support.

y is a locally stable equilibrium if there exists ϵ such that $E(y+u;y) \ge 0$ for all $\|Du\|_{\ell^2(\mathcal{B})} \le \epsilon$.

AIM: Find globally and locally stable equilibrium configurations containing dislocations.

Definition of a Dislocation





Use Algebraic Topology approach of Ariza-Ortiz (2005).

Cells: $\mathcal{C} := \{\mathrm{conv}\{\xi_1, \xi_2, \xi_3\} \,|\, (\xi_1, \xi_2), (\xi_2, \xi_3), (\xi_3, \xi_1) \in \mathcal{B}\}$
($=$ set of all triangles)

Can give an additive structure, and define boundary operators $\partial : \mathcal{C} \to \mathcal{B} \to \Lambda$ in a natural way.

Definition of a Dislocation

We can also define a notion of 'integration'.

- If $C = (\xi, \zeta, \eta) \in \mathcal{C}$, then

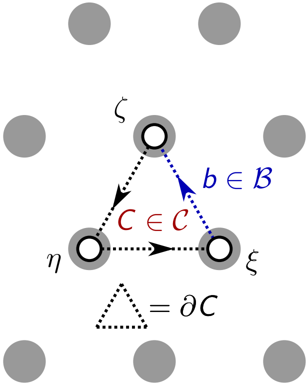
$$\int_{\partial C} \alpha = \alpha_{(\zeta,\xi)} + \alpha_{(\eta,\zeta)} + \alpha_{(\xi,\eta)}.$$

- Recall that $Dy = \alpha + z$,

$$0 = \int_{\partial C} Dy = \underbrace{\int_{\partial C} \alpha}_{\in[-\frac{3}{2},\frac{3}{2}]} + \underbrace{\int_{\partial C} z}_{\in\mathbb{Z}},$$

  and so $\int_{\partial C} \alpha \in \{0, \pm 1\}$.

- Think of $\int_{\partial C} \alpha$ as the **Burgers vector**.



Definition: $C \in \mathcal{C}$ is a dislocation core for y if $\int_{\partial C} \alpha \neq 0$.
Positive cores: $\mathcal{C}^+[y] := \{C \in \mathcal{C} \mid \text{+vely oriented}, \int_{\partial C} \alpha = 1\}$
Negative cores: $\mathcal{C}^-[y] := \{C \in \mathcal{C} \mid \text{+vely oriented}, \int_{\partial C} \alpha = -1\}$

Existence of a single dislocation

Theorem [TH, C Ortner]

Assume $\psi \geq \psi''(0)\psi_{\rm lin}$, then there exists a globally stable equilibrium y containing at least one dislocation.

Proof:

1. Define $\hat{y}(x) := \frac{1}{2\pi}\arg(x) = \frac{1}{2\pi}\arctan(x_2/x_1)$ [Remark: $D\hat{y} \notin \ell^2$]
   (branch cut along x_1)
   $\Rightarrow \quad \int_\Gamma \hat{\alpha} = 1$ for all closed curves Γ encircling the origin
2. $\mathcal{E}(u) := E(\hat{y} + u; \hat{y})$, $\dot{\mathscr{W}}^{1,2} := \{u : \Lambda \to \mathbb{R} \,|\, Du \in \ell^2\}$,
   $\Rightarrow \quad \mathcal{E} \in C(\dot{\mathscr{W}}^{1,2})$
3. Prove that $\mathcal{E}$ has a minimizer in $\dot{\mathscr{W}}^{1,2}$.
4. Let u be a minimiser; $y = \hat{y} + u$;
   $Du \in \ell^2 \quad \Rightarrow \quad \alpha = \hat{\alpha} + Du + z$, where z is compactly supported
   $\Rightarrow \quad \int_\Gamma \alpha = \int_\Gamma \hat{\alpha} = 1$

Existence of a single dislocation: Step 3 of Proof

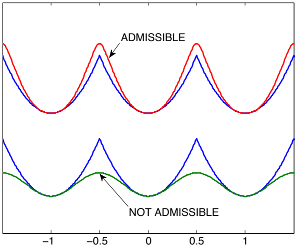
- $\hat{y}(x) := \frac{1}{2\pi} \arg(\xi) = \frac{1}{2\pi} \arctan(x_2/x_1)$ (branch cut along x_1)
- $\dot{\mathscr{W}}^{1,2} := \{u : \Lambda \to \mathbb{R} \,|\, Du \in \ell^2\}$
- $\mathcal{E}(u) := E(\hat{y} + u; \hat{y}) \qquad \Rightarrow \qquad \mathcal{E} \in C(\dot{\mathscr{W}}^{1,2})$

Theorem [TH, C Ortner]
Let $\psi \geq \psi''(0)\psi_{\rm lin}$, then there exists a global minimizer of $\mathcal{E}$ in $\dot{\mathscr{W}}^{1,2}$.

Strategy: Direct Method

Problem: Because $\mathcal{E}$ respects lattice symmetries, it is not coercive

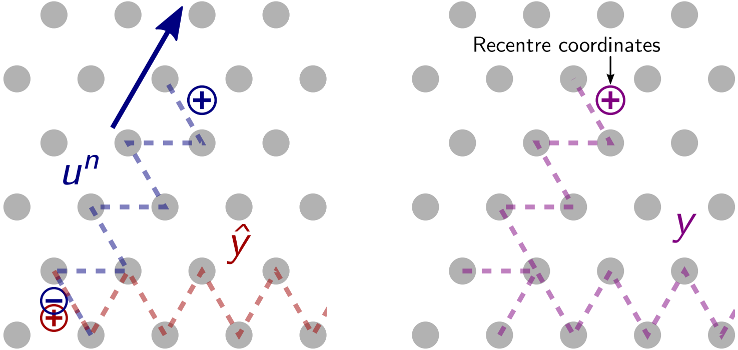
$$\mathcal{E}(u) = E(\hat{y} + u; \hat{y}) = \sum_{b \in \mathcal{B}} \Big(\psi(D\hat{y}_b + Du_b) - \psi(D\hat{y}_b) \Big)$$



Failures of compactness: Issues with dipoles

Failure of compactness 1: Dislocation 'Motion'

Cores translate to infinity along a minimising sequence.

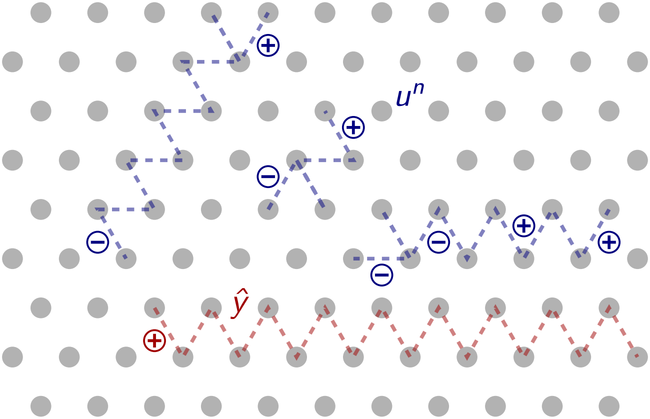


Resolution: Use translation invariance to recentre coordinates so dislocation core remains at the origin.

Failures of compactness: Issues with dipoles

Failure of compactness 2: Dislocation Multiplication

$\#\mathcal{C}^{\pm} \to \infty \rightsquigarrow$ MAIN DIFFICULTY; need to bound number of cores



Resolution: A concentration compactness principle: Lions (1985)

- Redefine minimising sequence with same energy but better properties
- Use structure to bound $\#\mathcal{C}^{\pm}$ for this sequence

Stability of general dislocation configurations

Stability Assumption (STAB): There exists $y = \hat{y} + u$, $u \in \dot{\mathscr{W}}^{1,2}$, $\delta\mathcal{E}(u) = 0$, and $\langle \delta^2\mathcal{E}(u)v, v\rangle \geq c_0\|Dv\|_2^2$ for all $v \in \dot{\mathscr{W}}^{1,2}$.

Remark: Can prove **(STAB)** directly for $\psi = \psi_{\rm lin}$. 'Expected' for globally stable configuration. In general, test numerically, see Ehrlacher-Ortner-Shapeev (2013).

Theorem [TH, C Ortner]

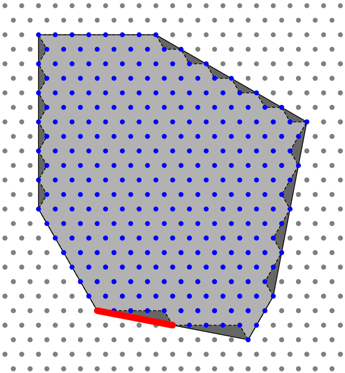
Suppose **(STAB)** holds, Ω is a convex lattice polygon or Λ, and $A \subset \mathcal{C}$ is a finite set such that $\mathcal{C}^{\pm}[\alpha] \subset A$.

For any $N \in \mathbb{N}$ there exist constants $L_0(N)$ and $S_0\big(N, \mathrm{index}(\partial\Omega)\big)$ such that whenever $(C_i, s_i) \in \mathcal{C}^{\Omega} \times \{-1, +1\}$, $i = 1, \dots, N$ with

- $\mathrm{dist}(C_i, C_j) \geq L_0(N)$, $i \neq j$, and
- $\mathrm{dist}(C_i, \partial\Omega) \geq S_0\big(N, \mathrm{index}(\partial\Omega)\big)$,

Then $\exists$ a locally stable configuration y' with $\mathcal{C}^{\pm}[\alpha'] \subset \bigcup_{i=1}^{N}(x^{C_i} + A)$ and $\int_{\partial(x^{C_i}+A)} \alpha' = s_i$.

Stability of general dislocation configurations



Proof of Theorem:

Inverse Function Theorem $\Rightarrow \exists$ local minimiser close to $z = \sum_i \hat{y}(\cdot - C_i) + \bar{y}_i + u(\cdot - C_i)$, where $\bar{y}_i$ is chosen to solve

$$-\Delta \bar{y}_i = 0 \text{ in } \Omega, \quad \frac{\partial \bar{y}_i}{\partial \nu} = -\frac{\partial}{\partial \nu}\hat{y}(\cdot - C_i) \text{ on } \partial\Omega.$$

Careful estimates on $\bar{y}_i$ and decay of u Ehrlacher-Ortner-Shapeev (2013) are needed to estimate $\delta\mathcal{E}^\Omega(z)$.

Remarks:

- S_0 depends only on the longest period in the boundary, not diam(Ω).
- $\hat{y}(\cdot - C_i) + \bar{y}_i =$ linear elasticity solution, $u(\cdot - C_i) =$ core corrector.
- If $\Omega = \Lambda$, dist$(C_i, \partial\Omega) := +\infty$, $\bar{y}_i \equiv 0$.
- Techniques could give energy asymptotics in terms of dist(C_i, C_j) and dist$(C_i, \partial\Omega)$, see also Alicandro-De Luca-Garroni-Ponsiglione (2013).

Conclusion

Summary:

- Anti-plane lattice model with natural symmetries: existence of globally stable configurations in infinite domain with unit Burgers vector
- Under stronger assumptions: locally stable configurations with arbitrary dislocation arrangement and in domains with polygonal boundaries

Outlook:

- Revival of study of dislocations in recent years: focus on connecting scales: molecular mechanics / meso-scale models $\rightsquigarrow$ semi-discrete point or line models $\rightsquigarrow$ dislocation density and plasticity models
- Our focus is on atomistic and atomistic to line/point models
  $\rightsquigarrow$ Next step: Stochastic atomistic dynamics $\rightarrow$ Continuum dynamics

References:

TH and C Ortner, Existence and stability of a screw dislocation under anti-plane deformation, *Arch. Ration. Mech. Anal.* 213(3):887–929 2014

TH and C Ortner, Analysis of stable screw dislocation configurations in an anti–plane lattice model, arXiv:1403.0518