Line Tension as the Dilute Limit of Discrete Dislocations

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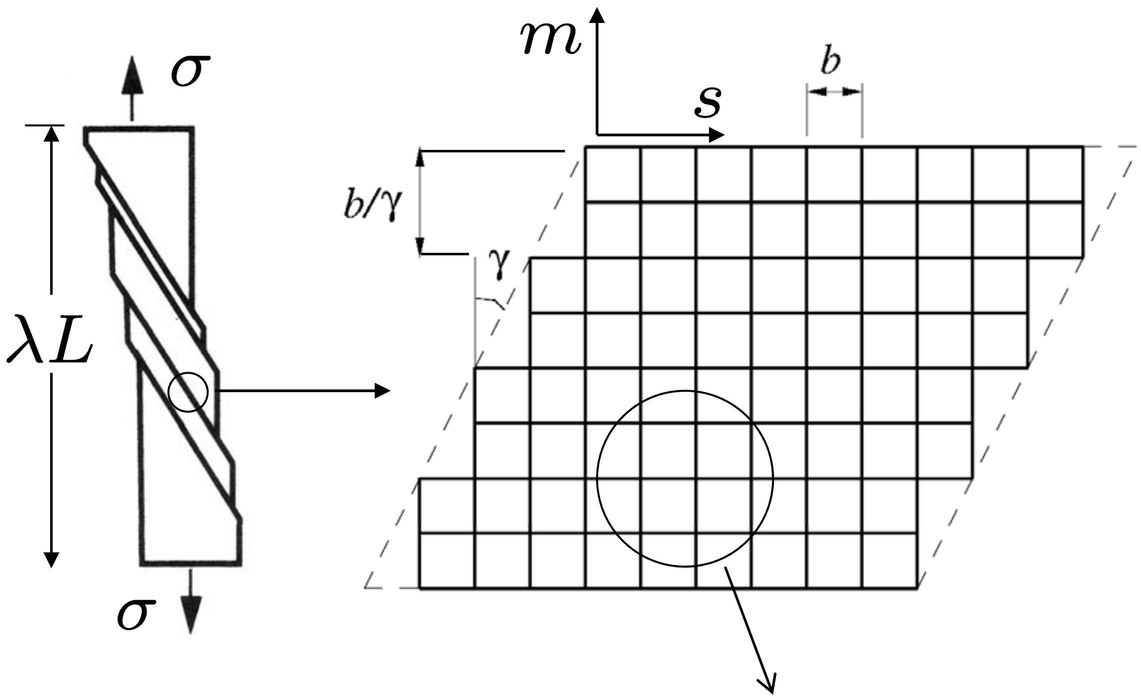
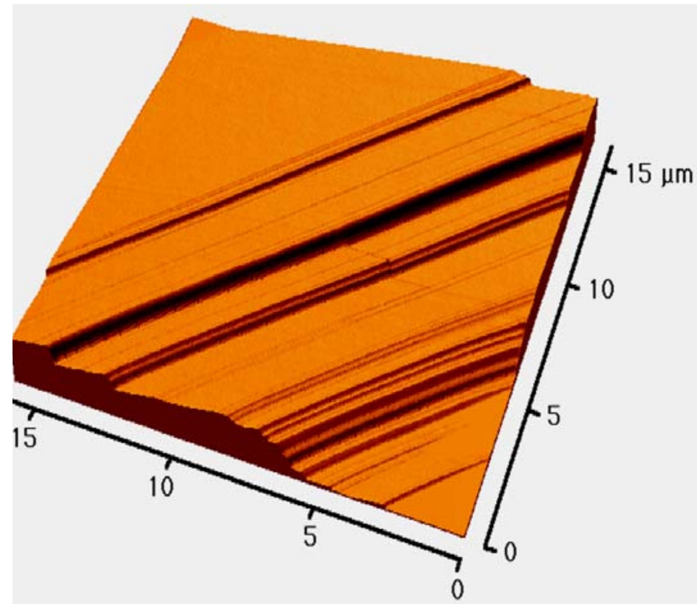
7^{th} International Congress on Industrial and Applied Mathematics (ICIAM11)
Vancouver, Canada
July 18-22, 2011

Introduction

- Linear-elastic dislocations in crystals: Energy is nonlocal, long-range elastic interactions
- Line-tension approximation: Energy ~ dislocation length
- Successful at describing kinetics of dislocation motion, hardening…
- Why does line-tension work?
- When does it work?

Discreteness of crystallographic slip



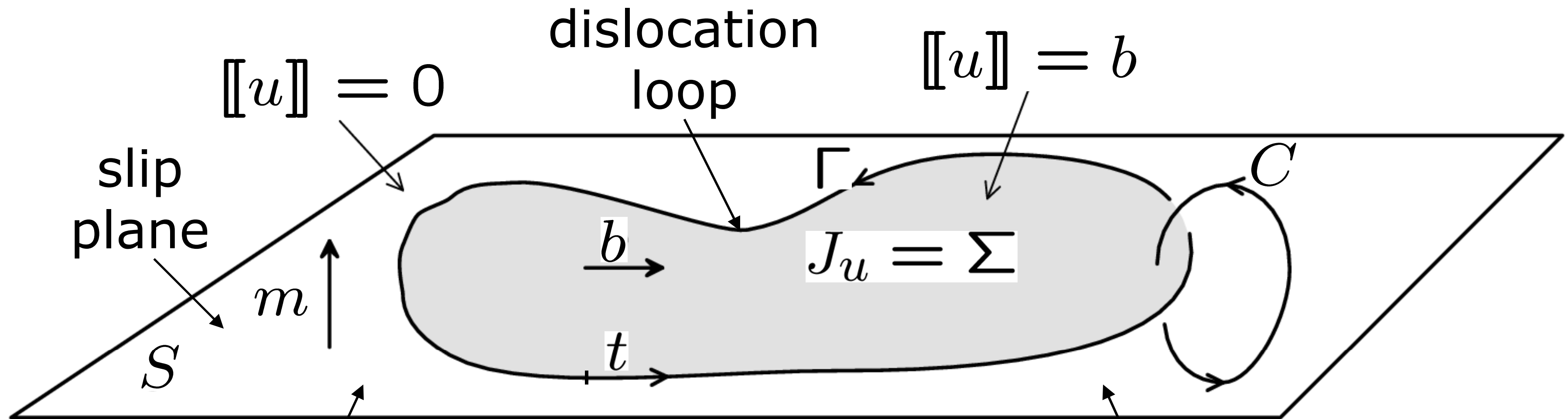


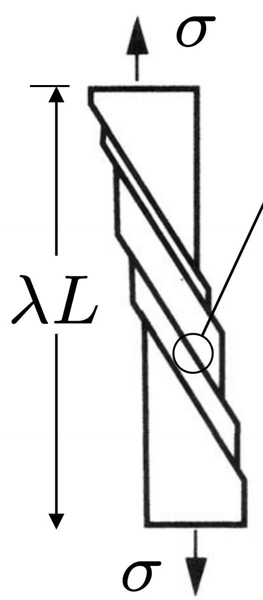
Crystallographic slip occurs on discrete slip planes characteristic of each crystal class

Crystallographic slip occurs through (low-energy) lattice-invariant deformations

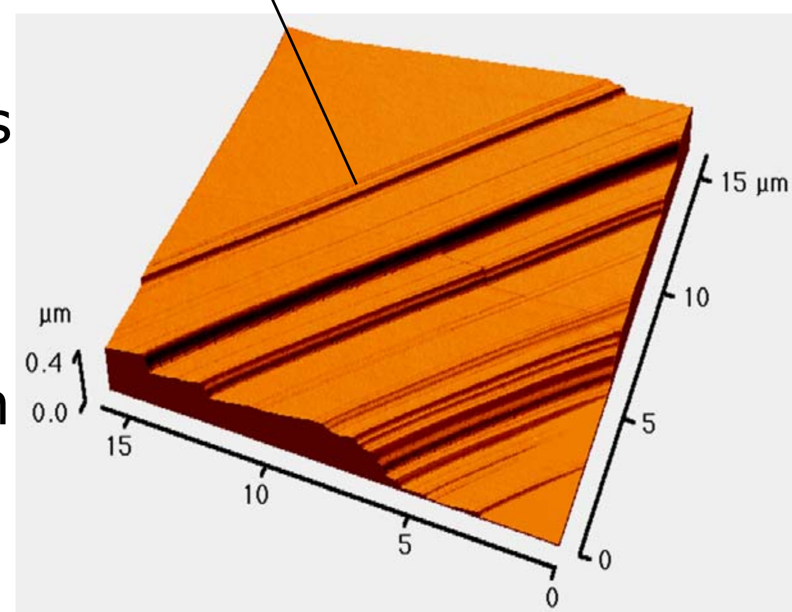
Slip traces on Cu crystal surface (AFM, C. Coupeau)

Crystallographic slip and dislocations

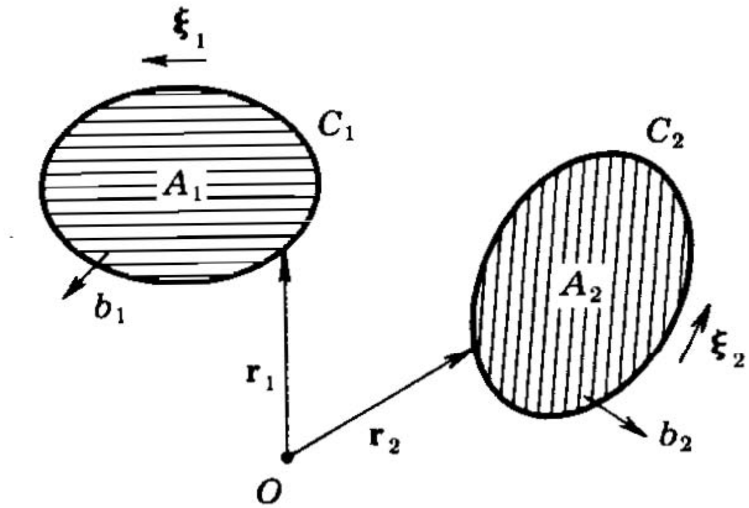




- Crystallographic slip occurs in discrete steps
- Locus of steps = dislocation lines
- Crystallographic slip proceeds by dislocation motion



Energy of linear-elastic dislocations



Two dislocation loops in an elastic crystal (Hirth & Lothe, 1982)

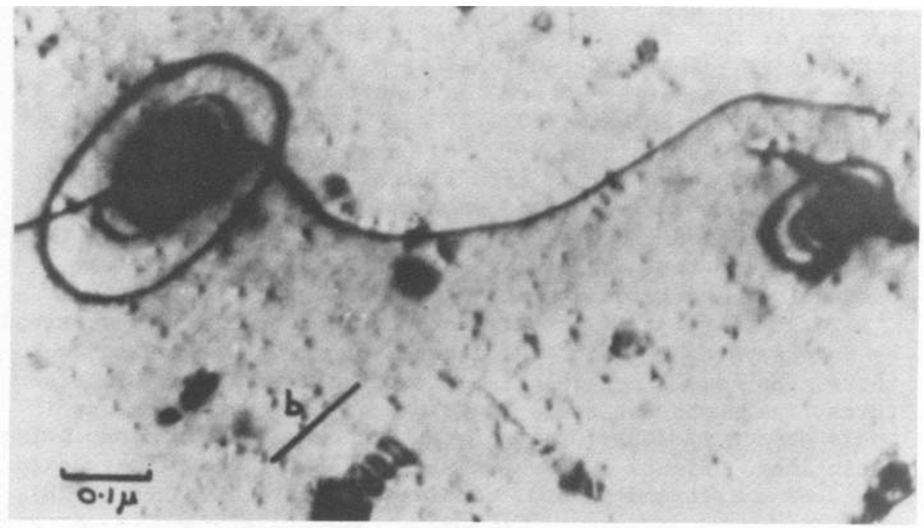
$$W_{12} = -\frac{\mu}{2\pi}\oint_{C_1}\oint_{C_2}\frac{(b_1\times b_2)\cdot(dl_1\times dl_2)}{R} + \frac{\mu}{4\pi}\oint_{C_1}\oint_{C_2}\frac{(b_1\cdot dl_1)(b_2\cdot dl_2)}{R} + \frac{\mu}{4\pi(1-\nu)}\oint_{C_1}\oint_{C_2}(b_1\times dl_1)\cdot T\cdot(b_2\times dl_2)$$

$$R = |r_1 - r_2|, \quad T_{ij} = \frac{\partial^2 R}{\partial x_i \partial x_j}$$

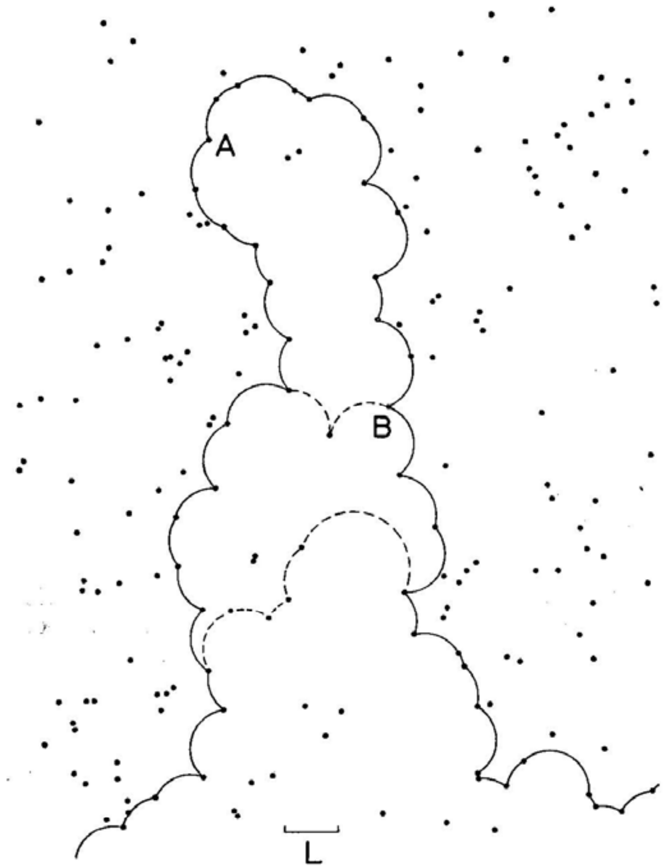
- All segment pairs interact through elastic field: $O(N^2)$!
- Self-energy of segments divergent logarithmically!

The line-tension approximation

- Approximate: $E \propto L$!



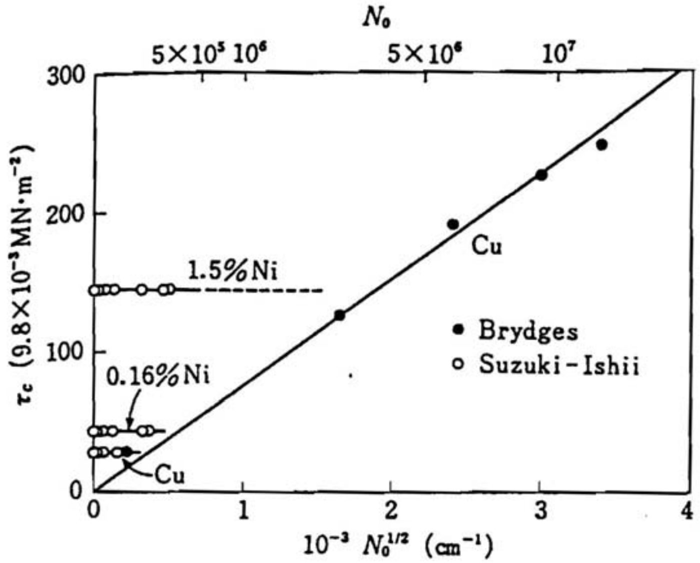
(Humphreys and Hirsch '70)

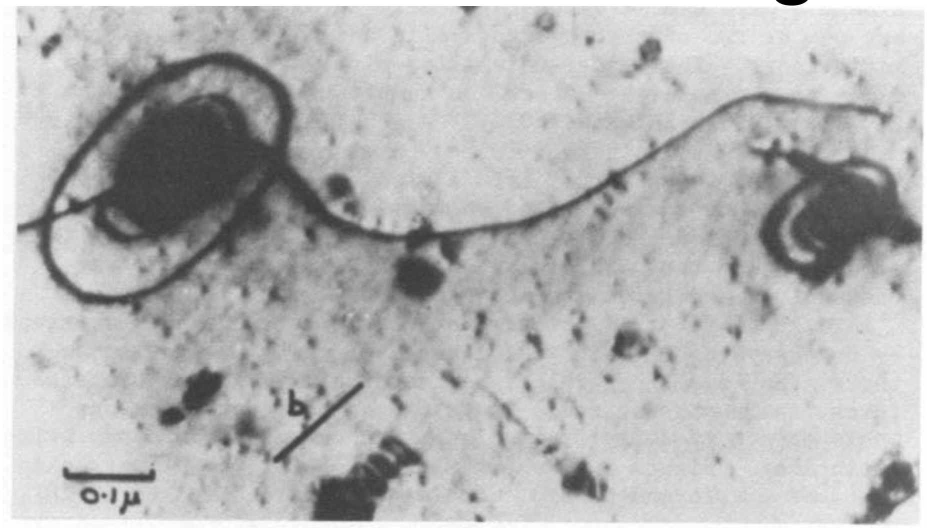


Dislocation motion through random obstacle array
(Foreman, A.J.E., Makin, M.J., *Phil. Mag.*, **14** (1966) 911)

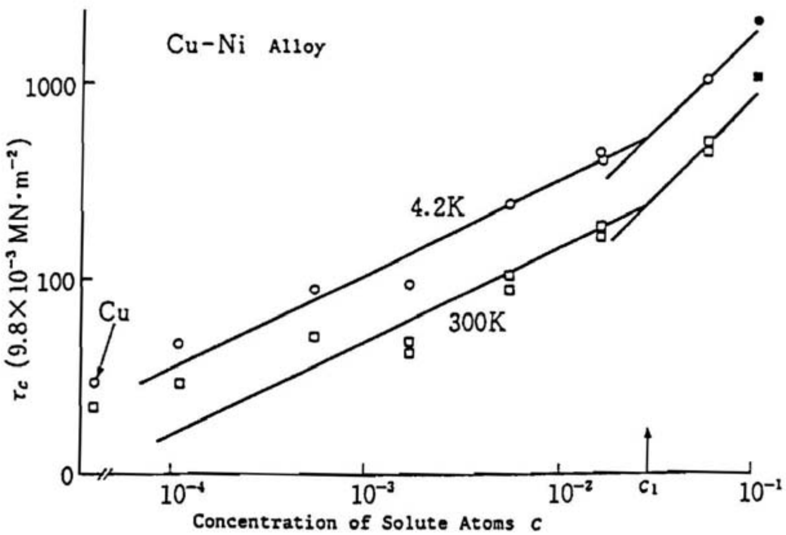
- Hardening: $\tau_c \sim c^{1/2}\gamma^{1/2}$, where:
  $c \equiv$ obstacle density, $\gamma \equiv$ slip strain

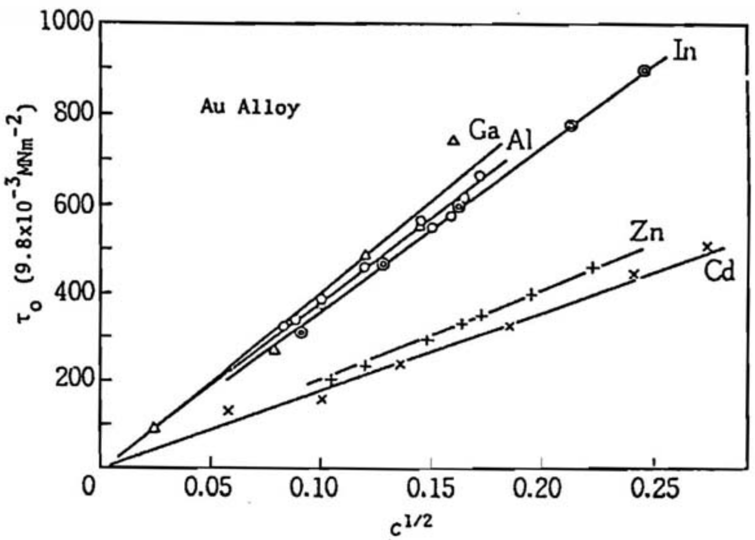
Line tension predicts observed scaling!





(Humphreys and Hirsch ’70)



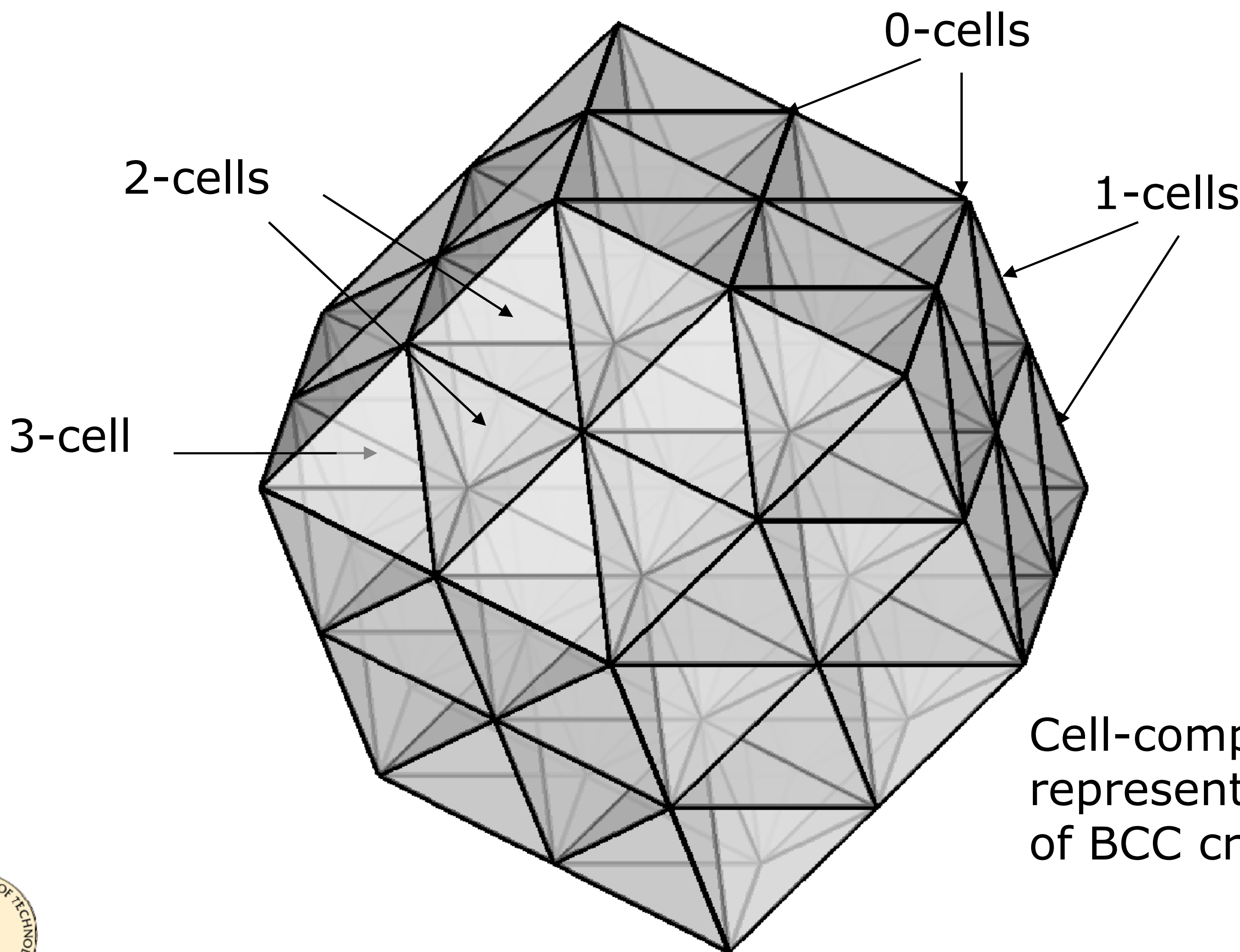


T. Suzuki, S. Takeuchi and H. Yoshinaga,
Dislocation Dynamics and Plasticity, Springer-Verlag, 1985.

Why does line tension work?

- The problem: To determine the low-energy configurations of linear-elastic dislocations
- The model: Discrete dislocations on discrete lattices interacting through discrete Green's functions (well-defined segment self-energies!)
- The results:
  1. *The asymptotic behavior of the stored energy in the* ***dilute limit*** *(in the sense of Γ-convergence) is given by the* ***line-tension approximation*** *(long-range interactions between dislocation segments can be neglected in the limit!)*
  2. ***Kinetic Montecarlo solver*** *based on the limiting energy*
  3. *Application* ***dislocation junctions***

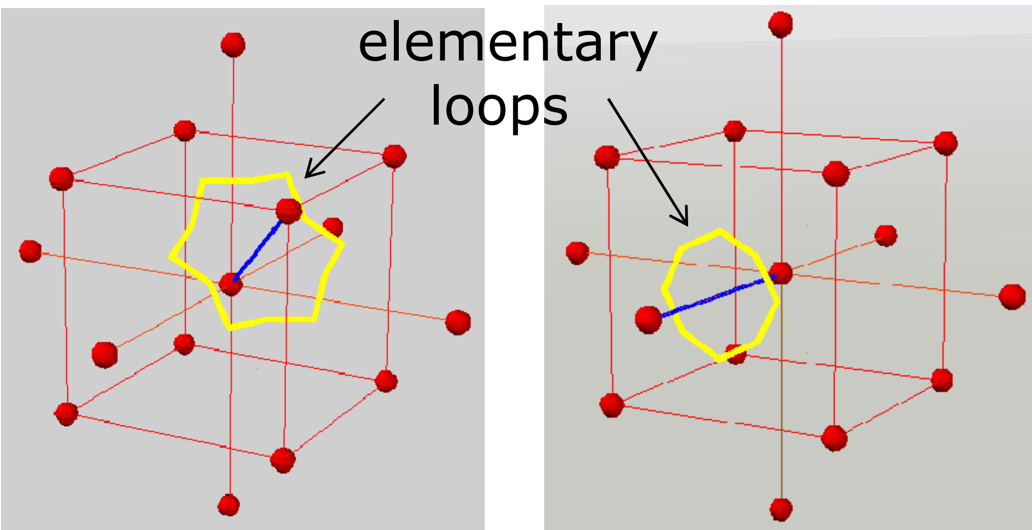
Lattice cell complexes

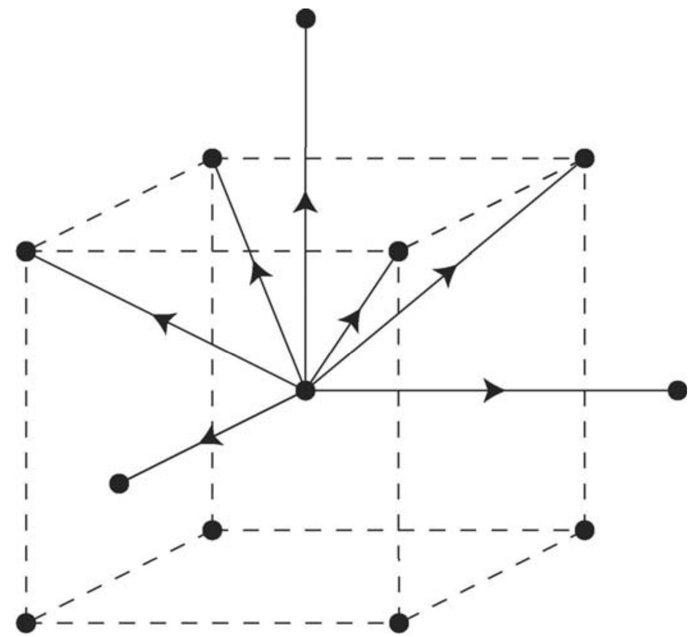


Cell-complex representation of BCC crystal

M.P. Ariza and M. Ortiz, *ARMA*, **178** (2005) 149–226.

Elementary dislocation loops



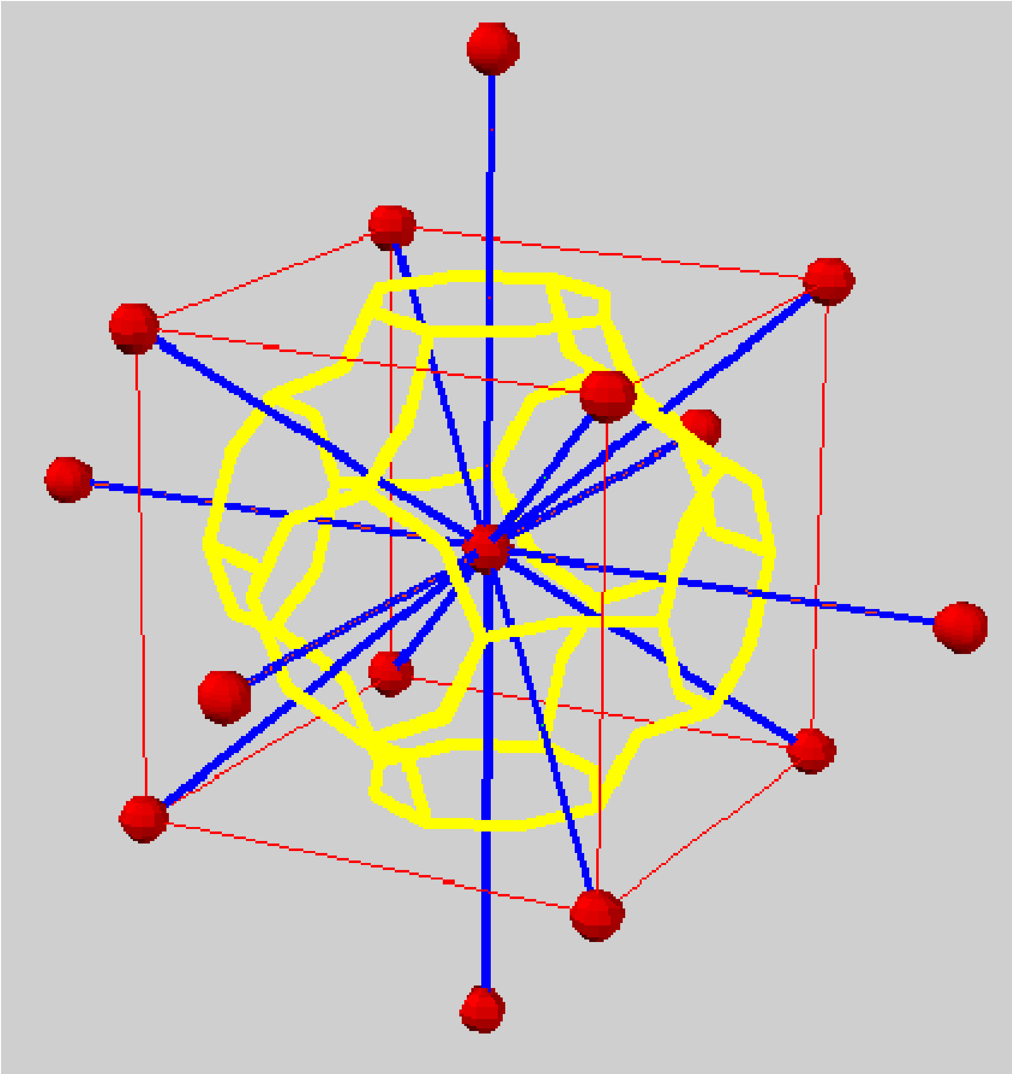


- Shown dislocation loops, their symmetry-group orbits and their translates form a basis for all closed discrete dislocation loops
- There is an elementary loop per atomic bond (1-cell) of lattice

- Atomic bonds (1-cells) of bcc lattice
- Bonds define 7 Bravais lattices (4 diagonal + 3 cubic atomic bonds)

- 7 types of elementary loops!

Elementary dislocation loops



bcc dislocation loop basis

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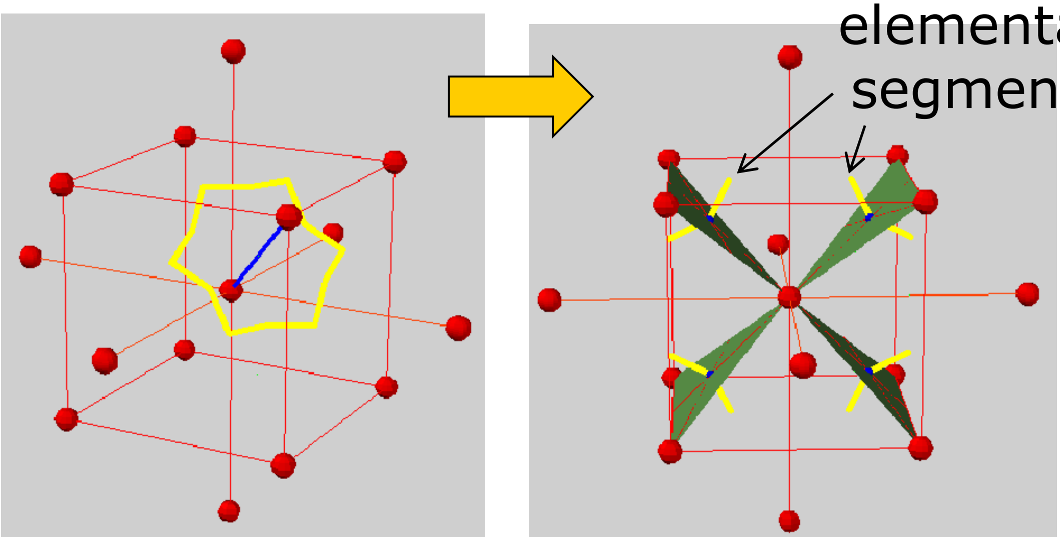
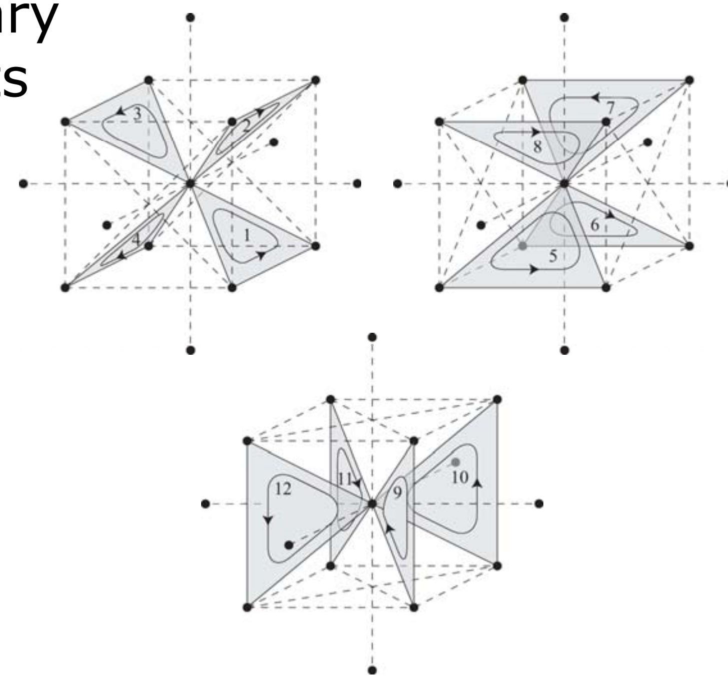
Elementary dislocation segments





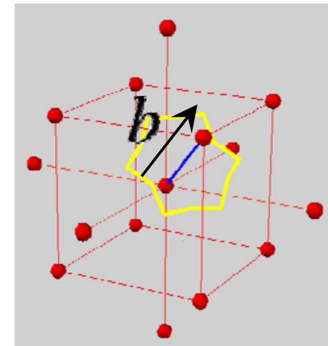
- Elementary dislocation loops can further be decomposed into elementary dislocation segments
- There is an elementary segment per face (2-cell) of lattice

- Face (2-cell) basis for bcc lattice
- Faces define 12 Bravais lattices

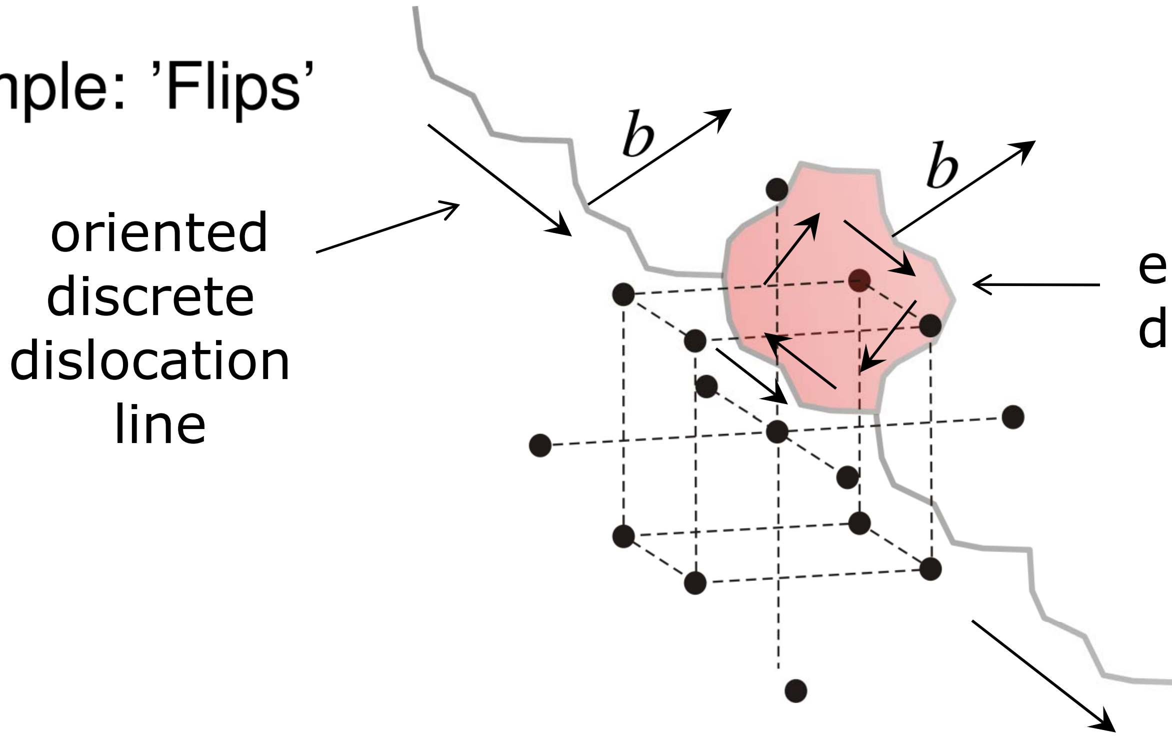
- 12 types of elementary segments!

Discrete dislocation densities

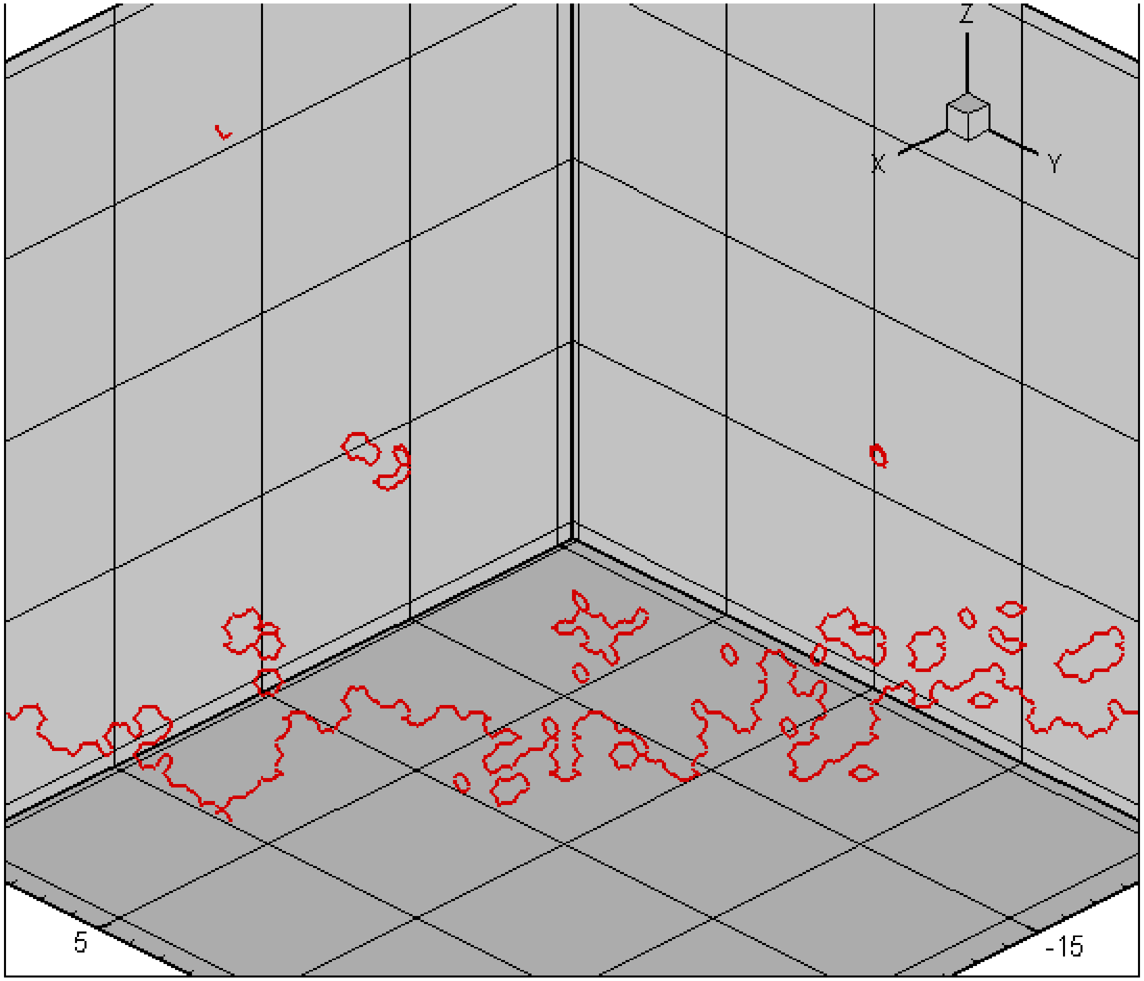
- Discrete dislocation density α:
  - Assign Burgers vectors to elementary loops
  - Add up algebraically all 'loaded' loops



- Example: 'Flips'



Discrete dislocation densities

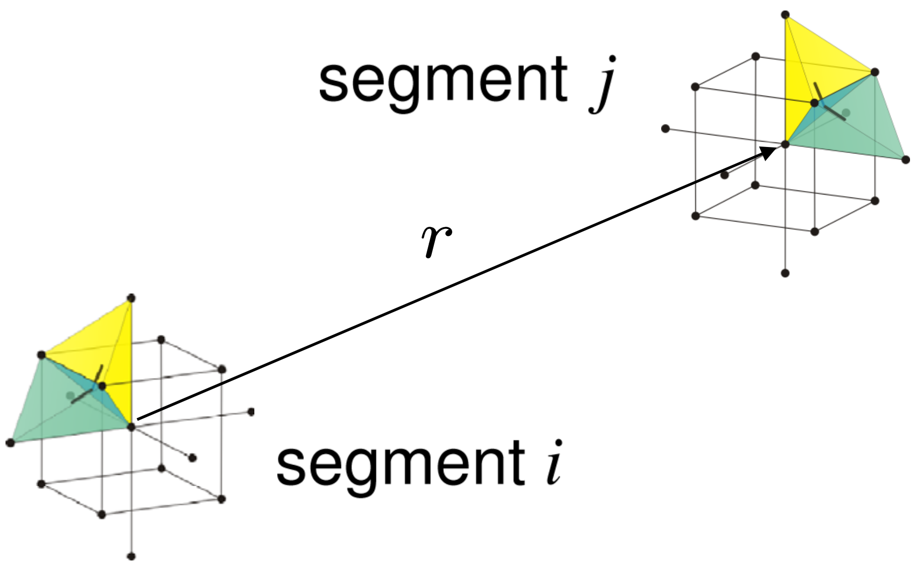


Complex discrete dislocation line generated through a sequences of flips

Discrete dislocations – Elastic energy

- Elastic energy: $E(\alpha) = \frac{1}{2}\sum_i \sum_j \langle \Gamma(x_j - x_i) b_i, b_j \rangle$

$\Gamma(r) \equiv$

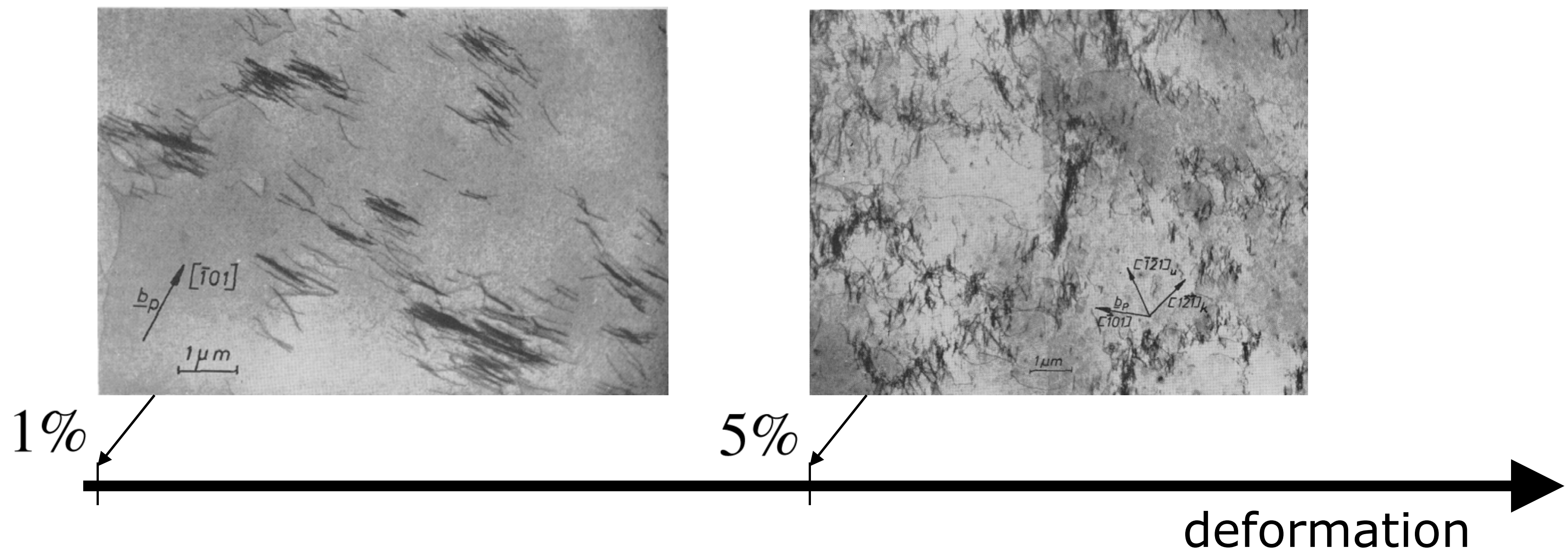


interaction energy between pair of elementary dislocation segments

- Kernel Γ follows from lattice force constants
- For large $|r|$, $\Gamma(r) \sim |r|^{2-n}$, $n \geq 3$; $\log |r|$, $n = 2$
- Long-range elastic interactions: $O(N^2)$!

Dislocation densities are dilute

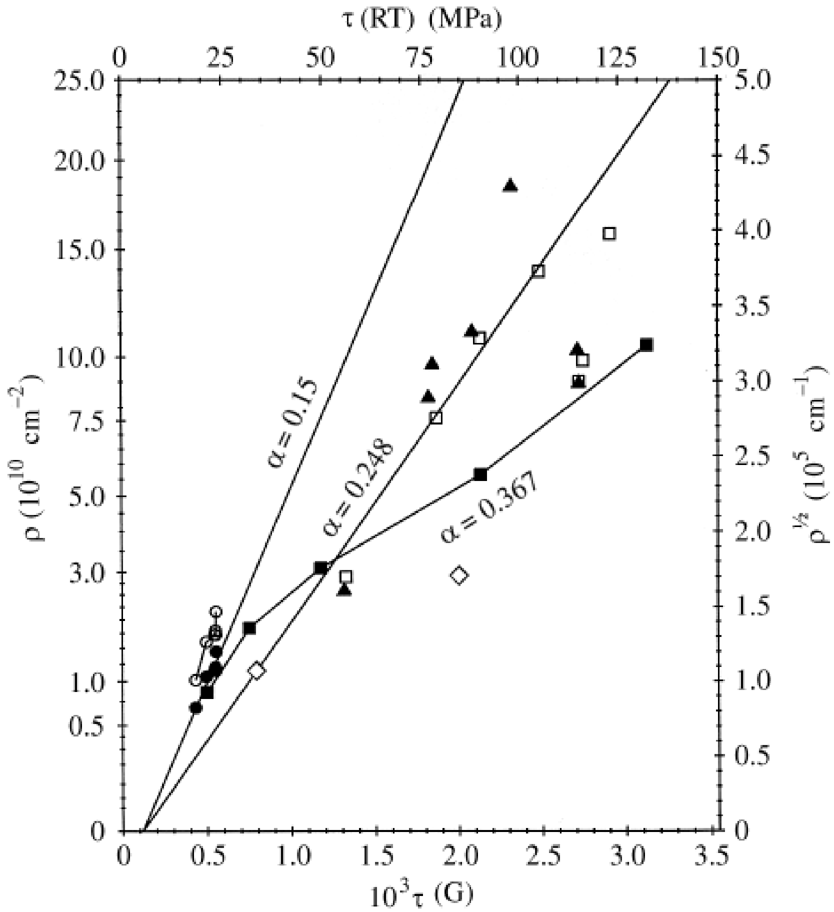
- Dislocation densities in plastically deformed crystals are fairly dilute, even at saturation
- Exploit this feature to simplify elastic energy!



Dislocations in
copper single crystal

H. Mughrabi, *Phil. Mag*. **23** (1971) 869

Dislocation densities are dilute

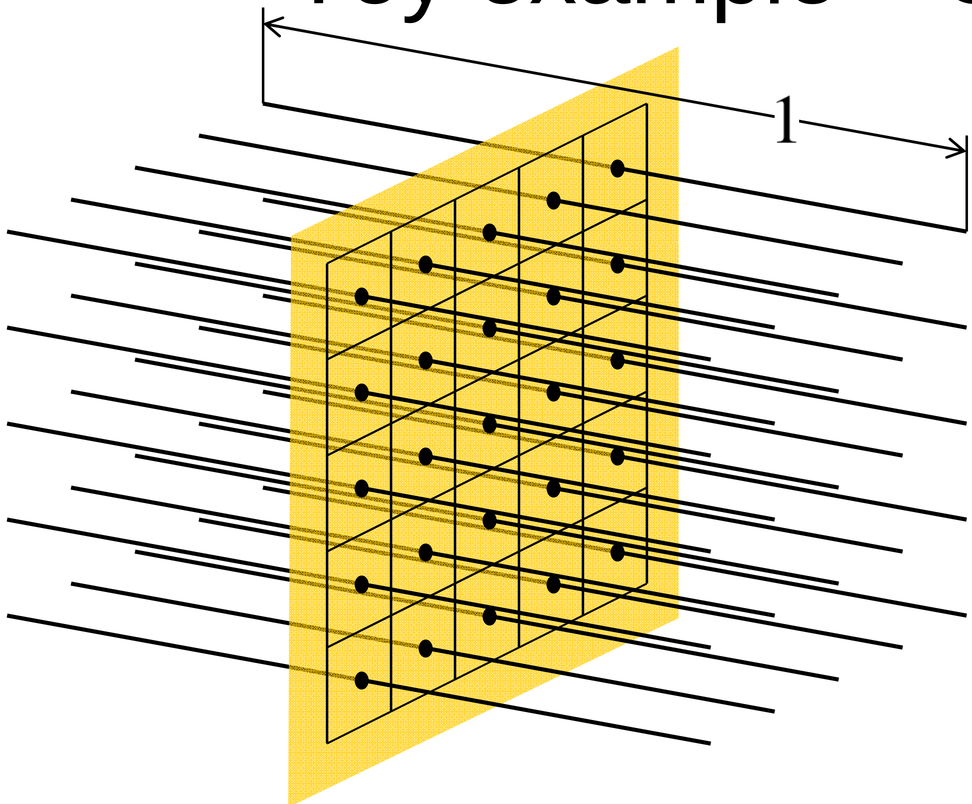


- Initial dislocation density ~ 10^{10} cm^{-2}
- Saturation dislocation density ~ 25 x 10^{10} cm^{-2}
- Initial mean distance between dislocations ~ 100 nm (278 lattice constants)
- Mean distance between dislocations at saturation ~ 20 nm (56 lattice constants)
- Investigate ***dilute limit***!

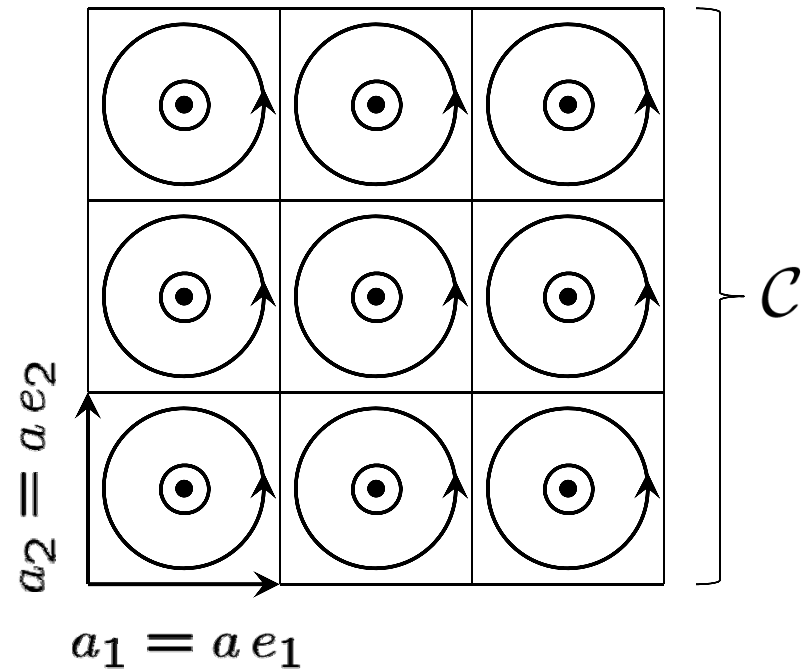
Total dislocation density *vs.* applied stress in single-crystal and polycrystalline copper in the deformation range of $\varepsilon \leq 0.4$

D. Breuer, P. Klimanek and W. Pantleon, *J. Appl. Cryst.*, **33** (2000) 1284-1294.

Toy example – Square lattice



Screw-dislocation bundle



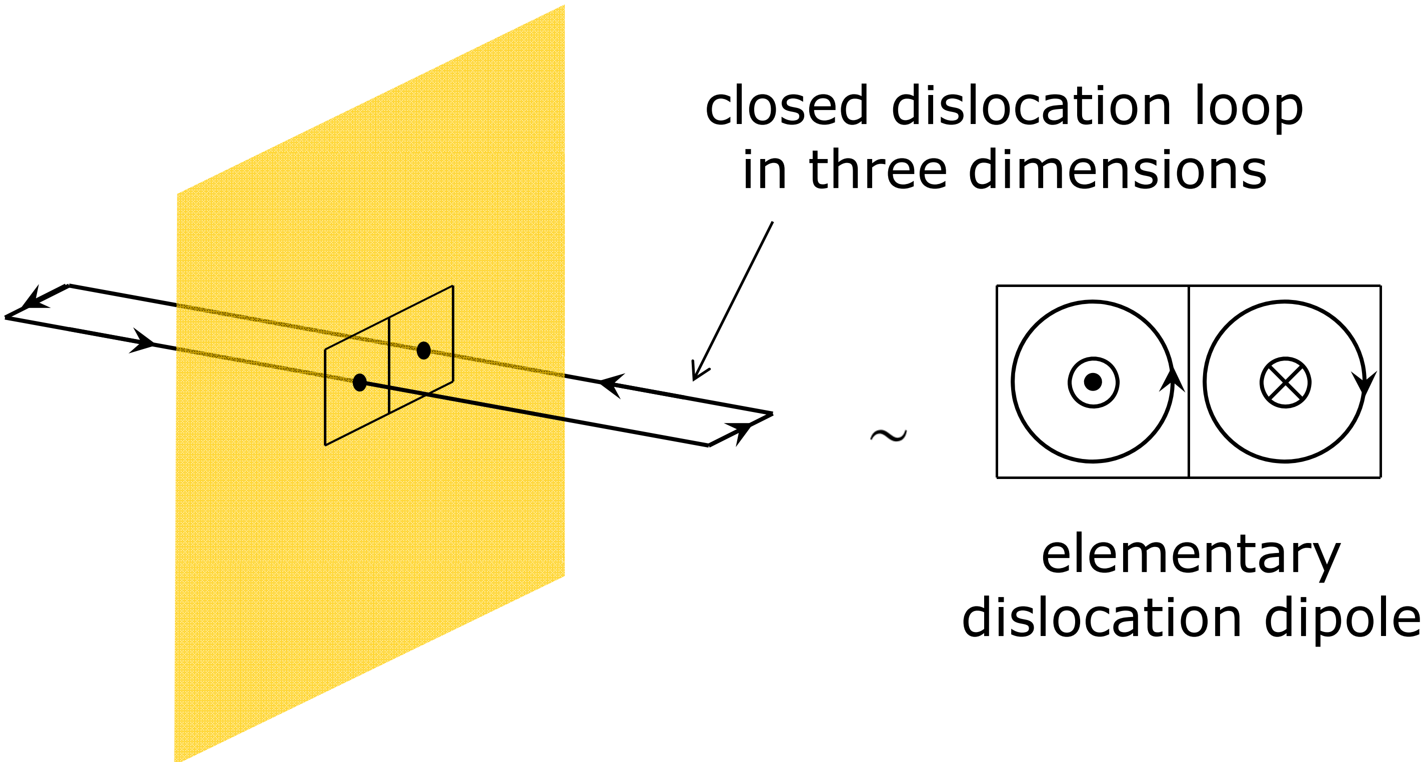
Square lattice complex

- Discrete dislocations (2-forms over $\mathcal{C}$):

$$\mathcal{D}^2(C;\mathbb{R}) \equiv \{\alpha = \sum_{r\in a\mathbb{Z}^2} b_r \delta_r,\ b_r \in \mathbb{R}\}$$

- Coboundary operator (div): $d\alpha = \sum_{r\in a\mathbb{Z}^2} b_r = 0!$

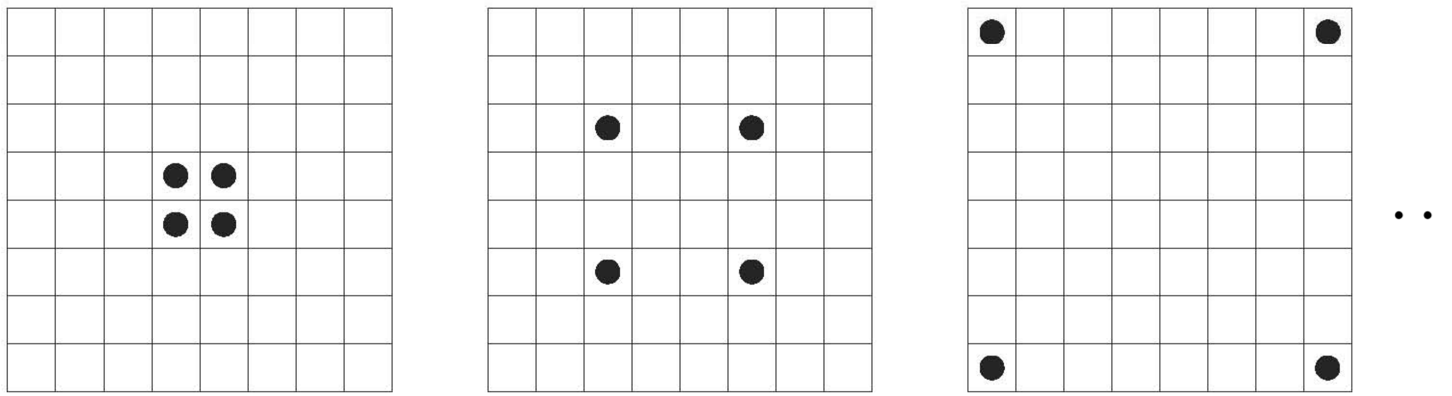
Toy example – Square lattice



- Dislocation dipole: $d\alpha = \sum_{r \in a\mathbb{Z}^2} b_r = b - b = 0$
- If $d\alpha = 0 \Rightarrow \alpha$ linear combination of elementary dipoles
- Discrete Helmholtz decomposition theorem!

M.P. Ariza and M. Ortiz, *ARMA*, **178** (2005) 149–226.

The dilute limit – Scheme I

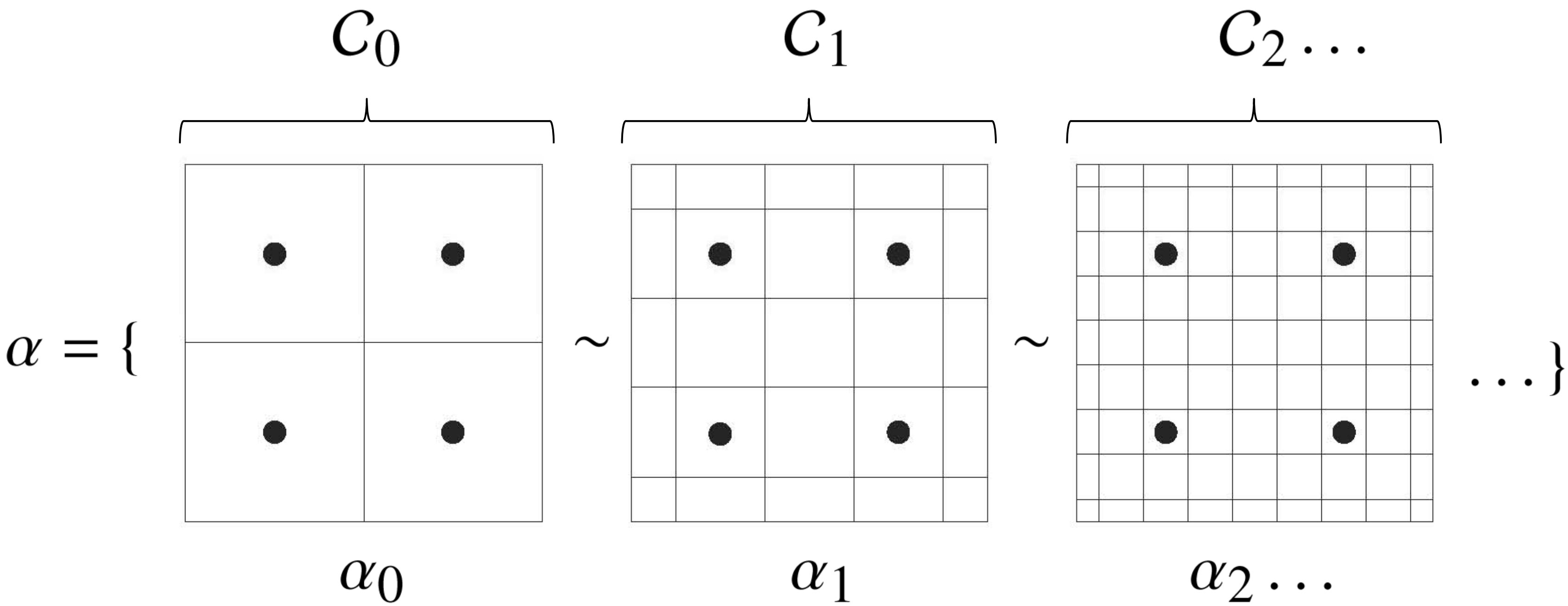


α_0 α_1 $\alpha_2 \ldots$

Sequence of increasingly ***dilute*** quadrupoles

- Weak limit: $\langle \alpha_h, \varphi \rangle \to 0$, $\forall$ test functions $\varphi \Rightarrow \alpha_h \rightharpoonup 0$!
- All dislocations 'go off' to infinity in the limit!

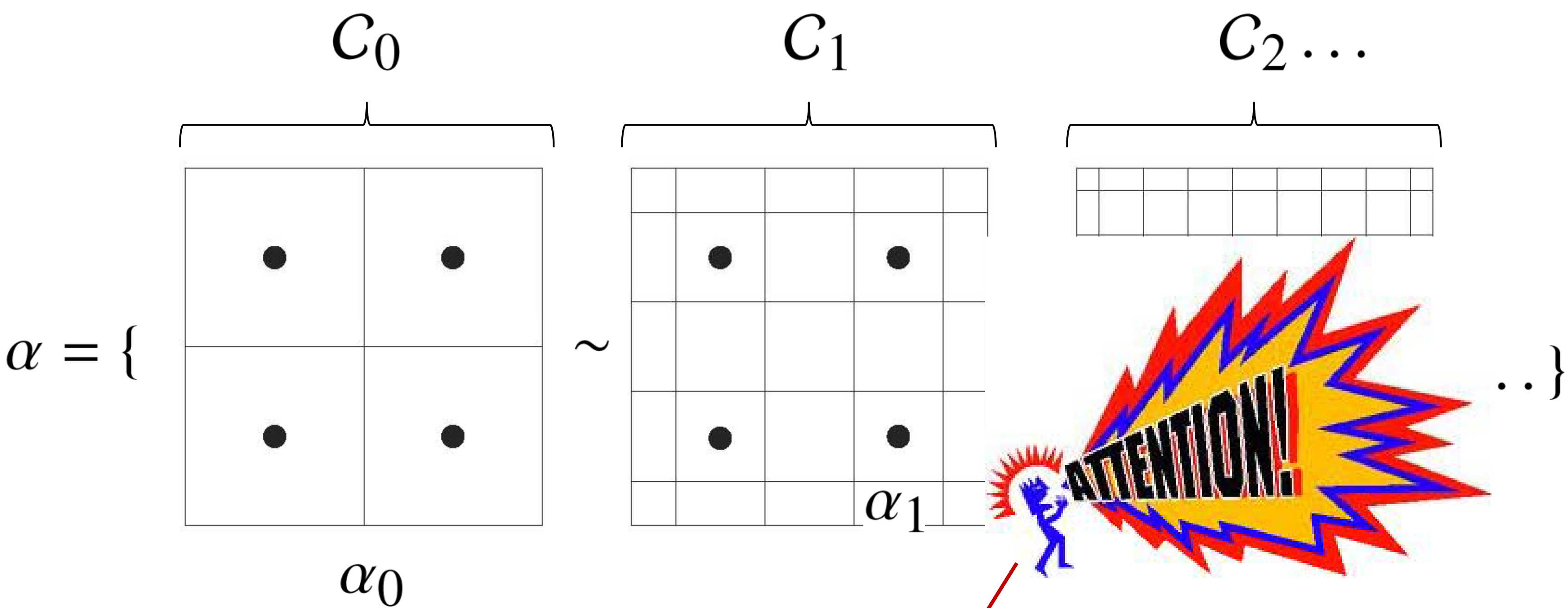
The dilute limit – Scheme II



Sequence of increasingly ***dilute*** quadrupoles

- Lattice refinement $\Rightarrow C_h,\ a_h = \epsilon_h a,\ \epsilon_h = 2^{-h},\ h \in \mathbb{N}$
- Identify $\alpha_0 \sim \alpha_1 \sim \alpha_2 \ldots \Rightarrow$ dilute dislocation!

Square lattice – Dilute dislocations

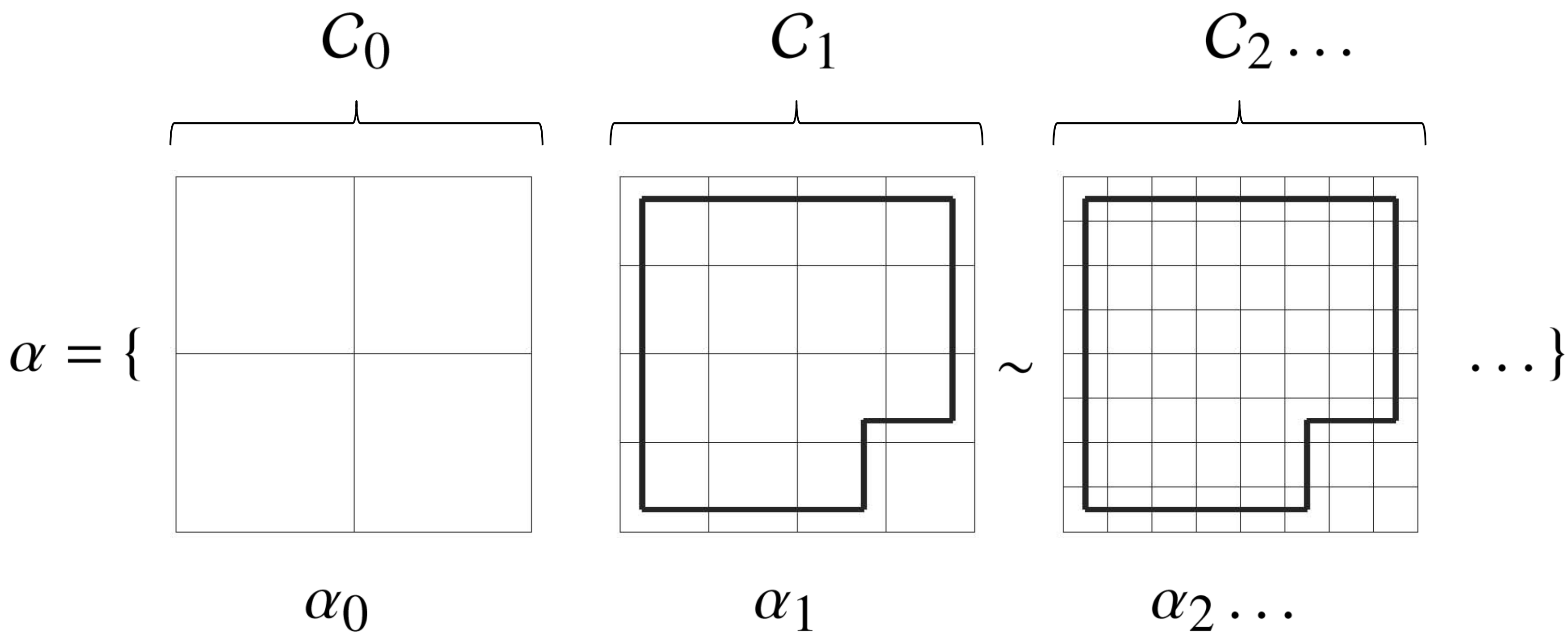


Sequence of increasingly ***dilute*** quadrupoles

- Space of DDDs: $X = \{\alpha = \sum_{r \in a\mathbb{Q}^2} b_r \delta_r, \ \|\alpha\| < +\infty\}$
- Inner product: $\langle \alpha', \alpha'' \rangle = \sum_{r \in a\mathbb{Q}^2} b'_r b''_r$
- Coboundary operator: $d\,\alpha = \sum_{r \in a\mathbb{Q}^2} b_r$

J.R. Munkres, *Elements of Algebraic Topology*, Perseus (1984)

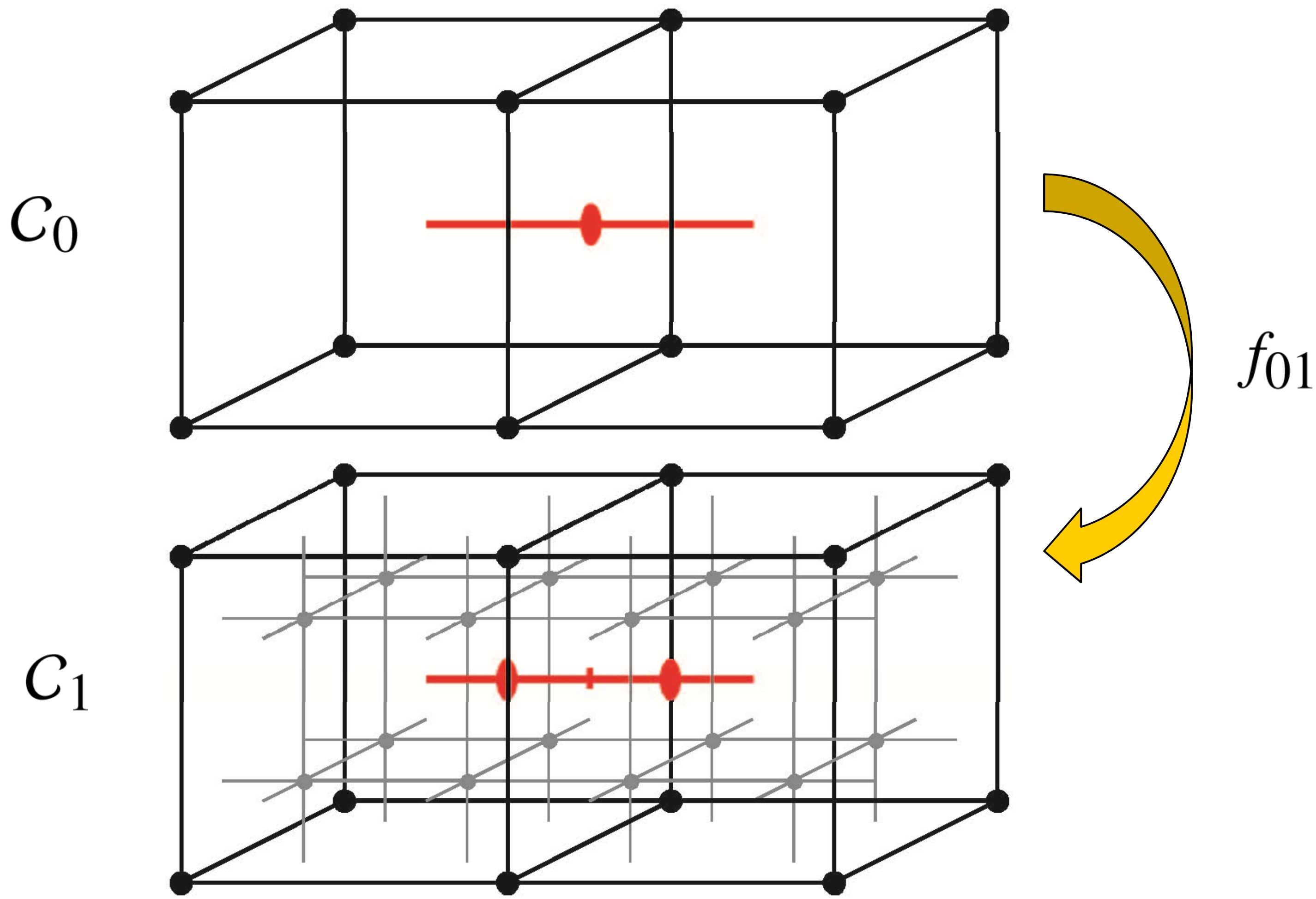
The dilute limit – Scheme II



Sequence of increasingly ***dilute*** dislocation loops

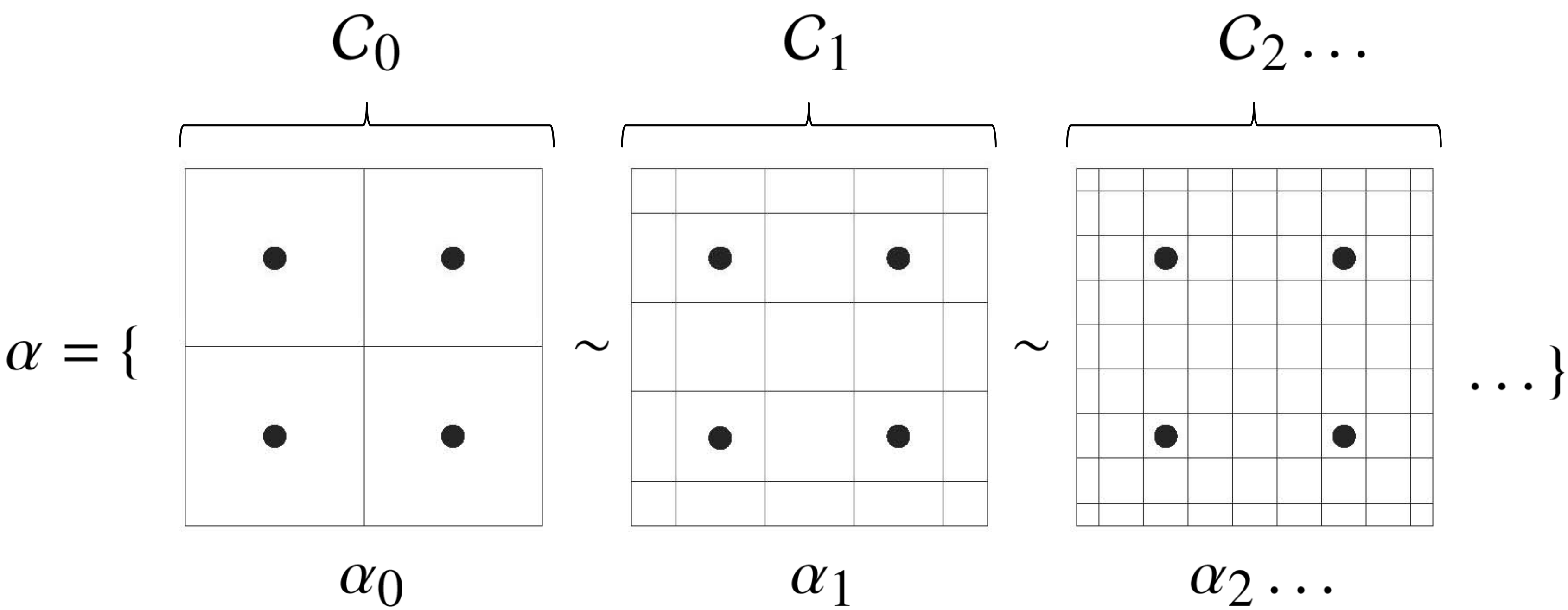
- Lattice refinement $\Rightarrow C_h$, $a_h = \epsilon_h a$, $\epsilon_h = 2^{-h}$, $h \in \mathbb{N}$
- Identify $\alpha_0 \sim \alpha_1 \sim \alpha_2 \ldots \Rightarrow$ dilute dislocation!
- Norm: $\|\alpha\|^2 = \epsilon_h \sum_r |b_{hr}|^2$, independent of h

The dilute limit – Scheme II



Segment refinement for cubic lattice

The dilute limit – Scheme II

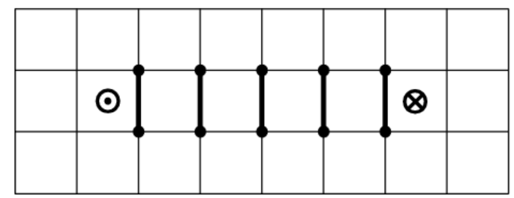


Sequence of increasingly ***dilute*** quadrupoles

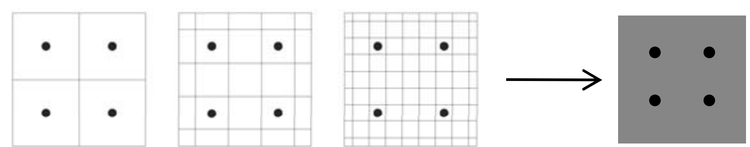
- For every dilute dislocation density (DDD), there is a sufficiently fine lattice that carries it
- The space of DDDs ~ l^2

The dilute limit – Line tension

- Refinement generates a sequence of energies $E_h(\alpha)$
- Expect $E_h(\alpha)$ to diverge as $\epsilon_h^{2-n} \log \epsilon_h^{-1}$
- Example: dipole, $E_h \sim \dfrac{\mu b^2}{2\pi} \log \epsilon_h^{-1}$



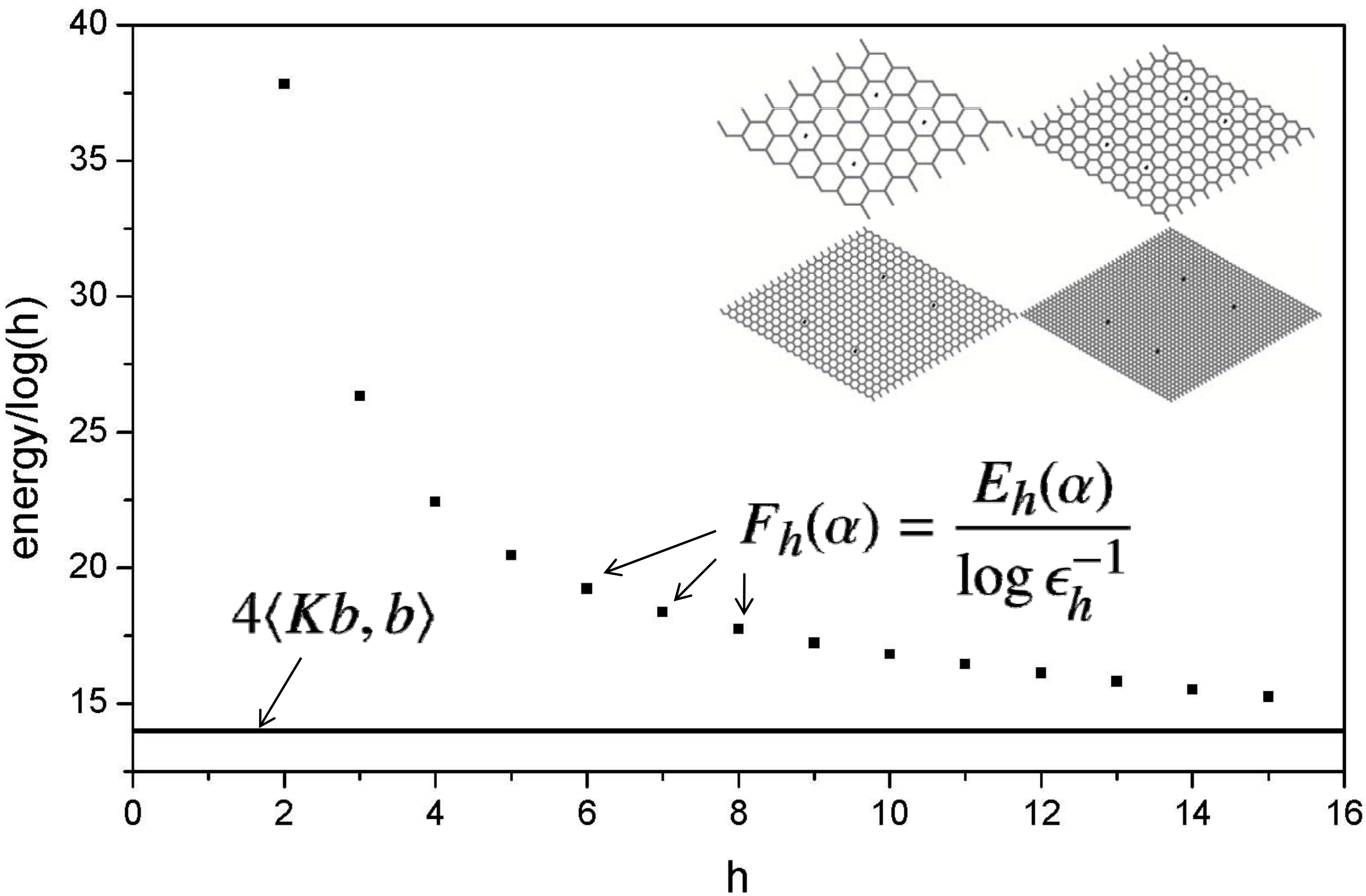
- Scaled energy: $F_h(\alpha) = \dfrac{1}{\epsilon_h^{2-n} \log \epsilon_h^{-1}} E_h(\alpha)$
- Question: $\Gamma\text{-}\lim_{h\to\infty} F_h$?



Thm $\Gamma\text{-}\lim_{h\to\infty} F_h = \underbrace{\sum_r \langle K b_r, b_r \rangle}_{\text{prelogarithmic energy factor}}$ (wrt weak convergence)

- No long-range interactions in limit $\Rightarrow$ Line tension!

Example – Graphene quadrupole



M.P. Ariza, M. Ortiz and R. Serrano,
Int. J. Fracture (2010) DOI 10.1007/s10704-010-9527-0

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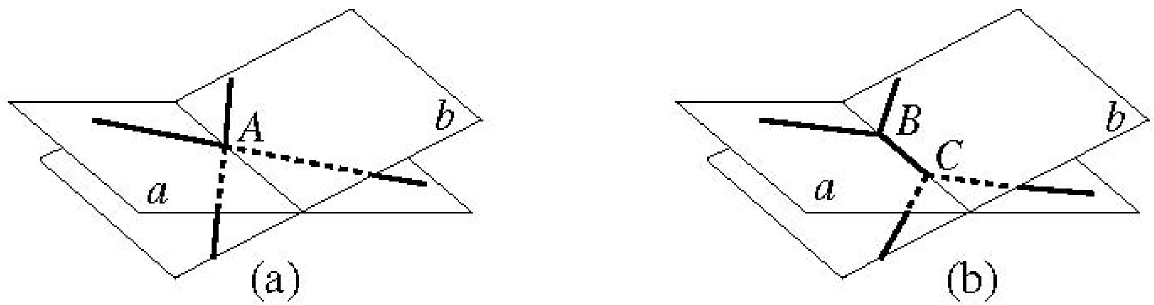
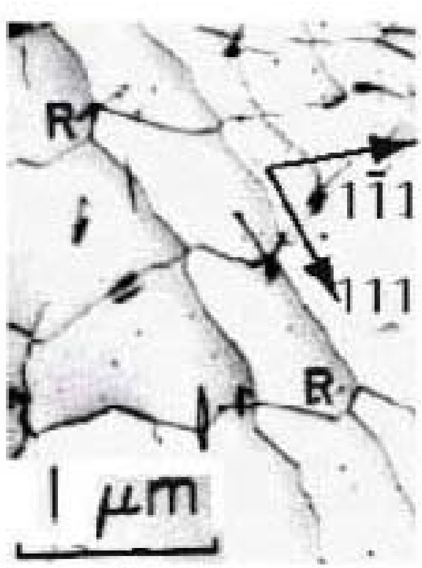
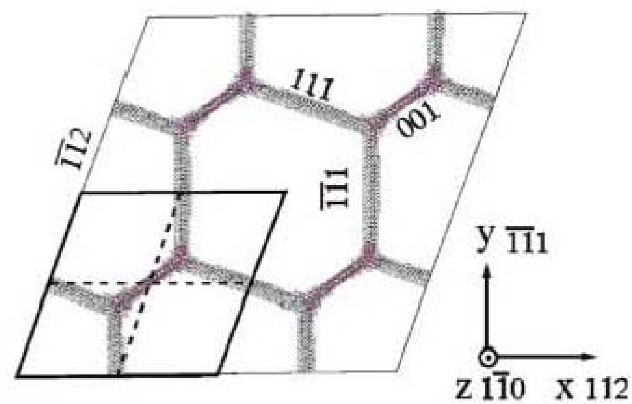
Line tension – Dislocation junctions



a) Dislocation lines on planes *a and b* collide at *A.*
b) Junction bounded by two 3-nodes *B and C is formed.*



Network of ½<111> screw dislocations forming <001> screw junctions

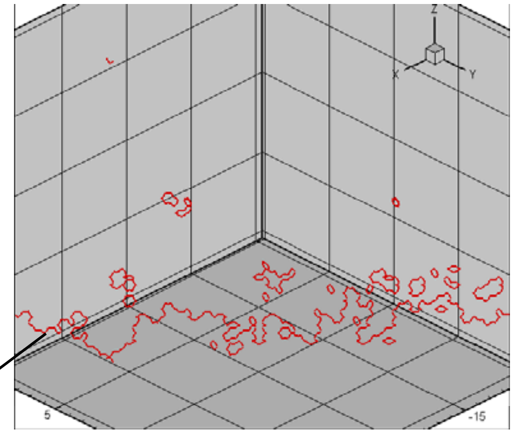


Atomistic simulations of Bulatov and Cai (2002)

V.V. Bulatov and W. Cai, *PRL*, **89** (2002) 115501.
H. Matsui and H. Kimura, *Mater. Sci. Eng*., **24** (1976) 247 .

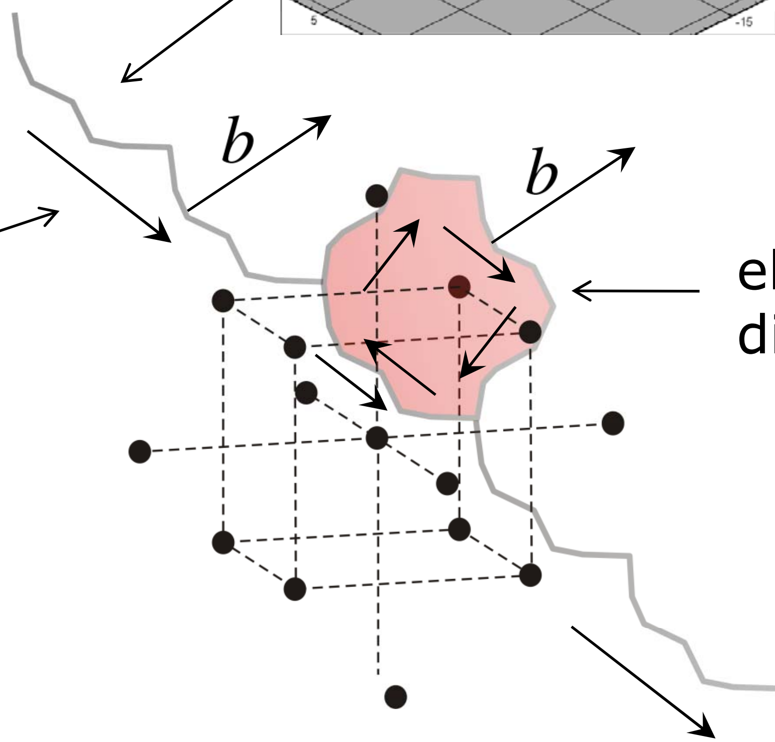
Kinetic Monte Carlo implementation

accept or
reject based on
line-tension!



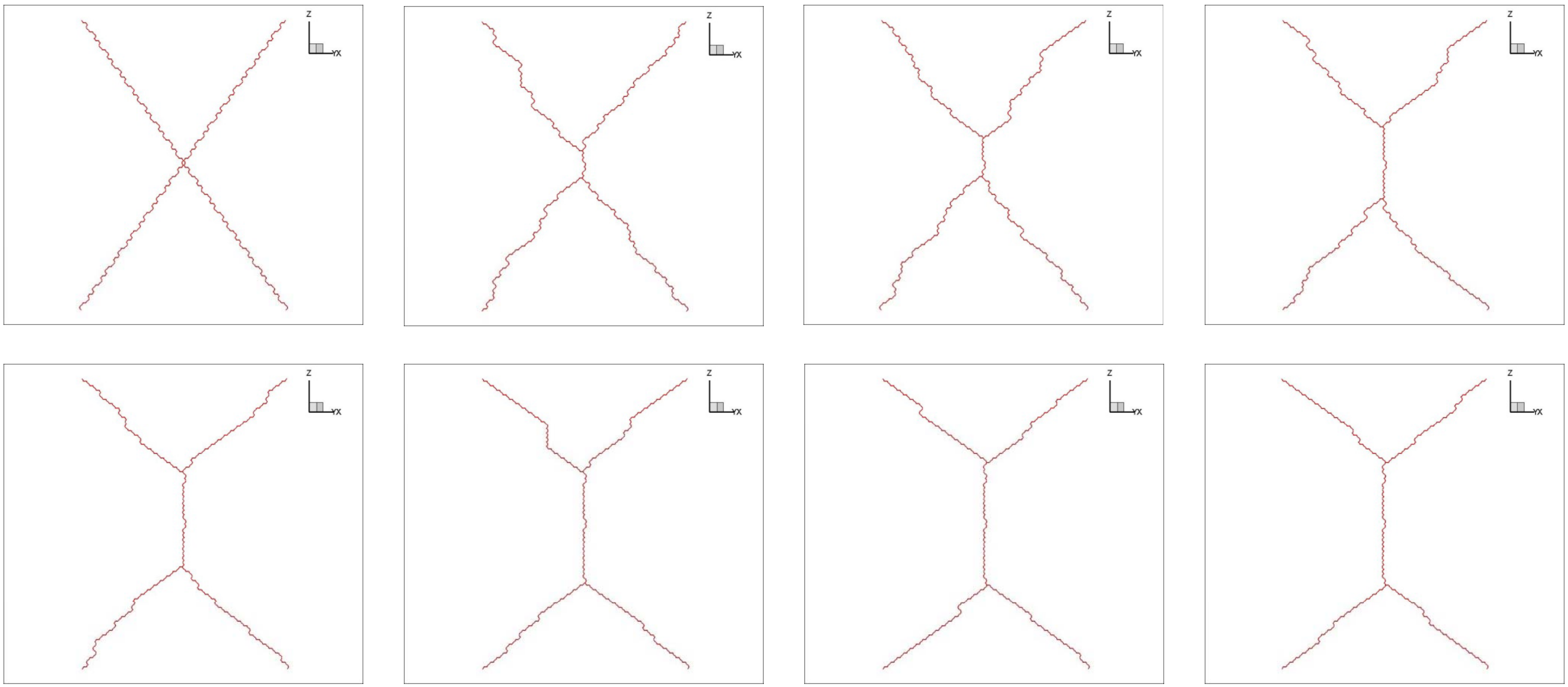
- 'Flips:'

oriented
discrete
dislocation
line



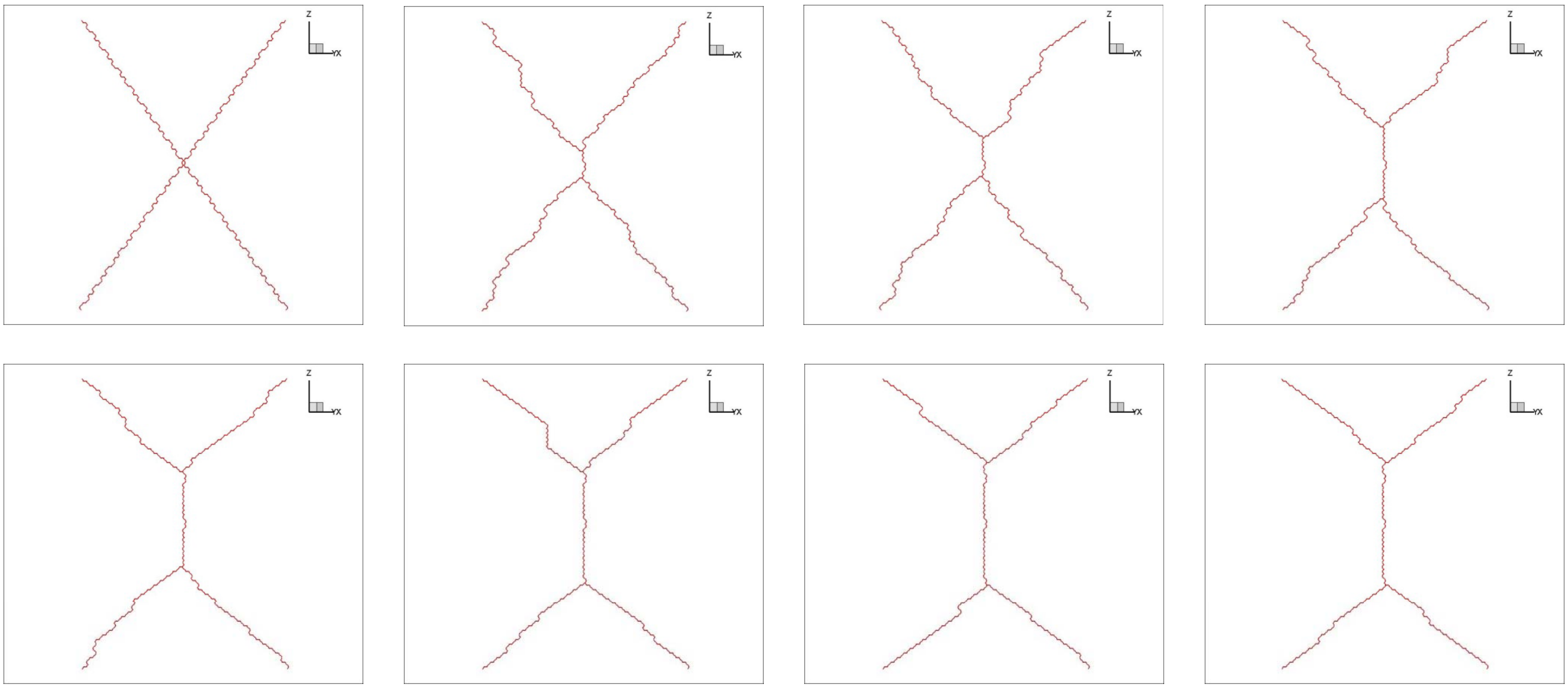
oriented
elementary
dislocation
loop

Energy-minimizing junction configuration



Snapshots of kMC calculation of energy minimizing configuration of junction, using line-tension approximation

Energy-minimizing junction configuration



Snapshots of kMC calculation of energy minimizing configuration of junction, using line-tension approximation

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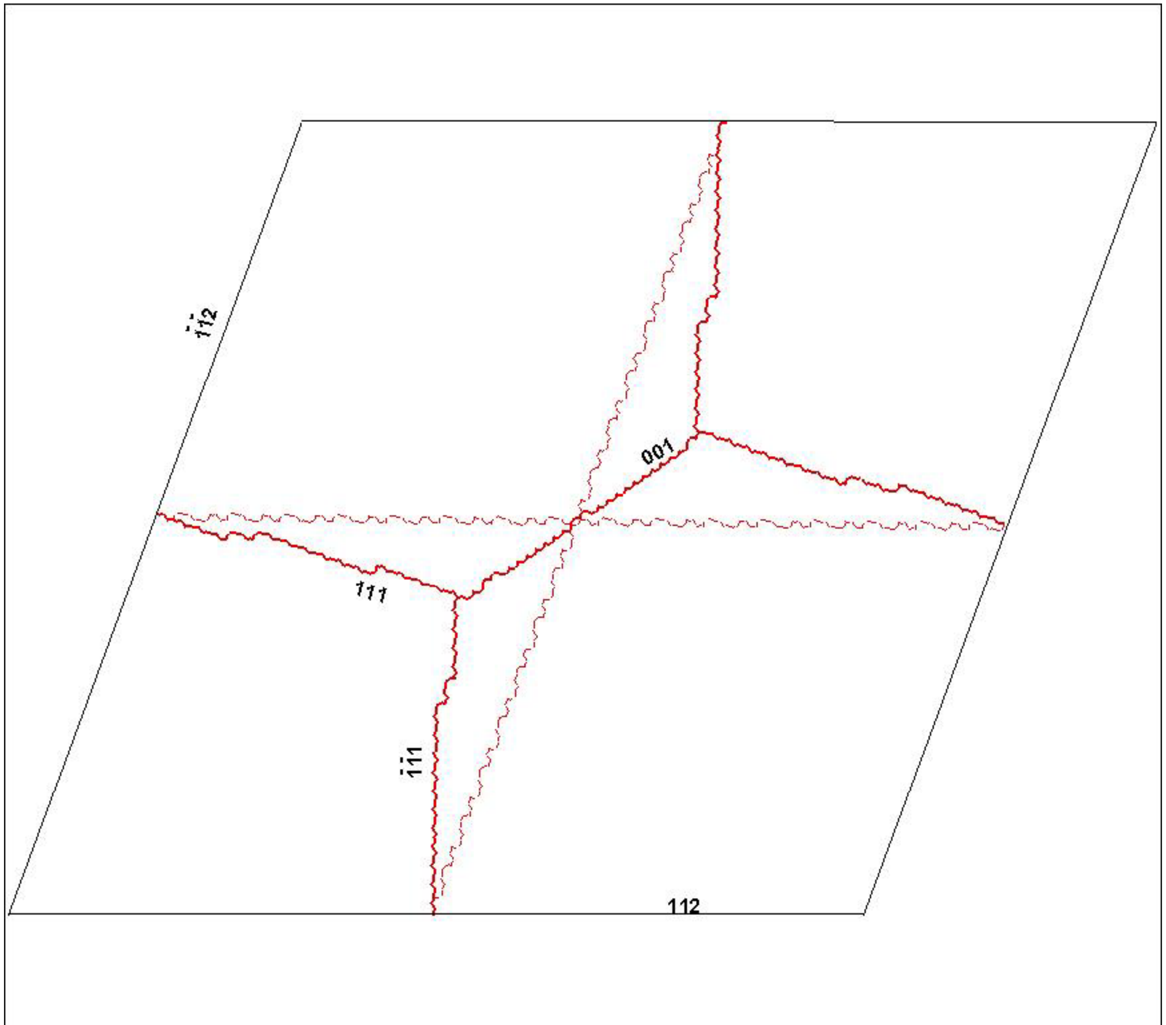
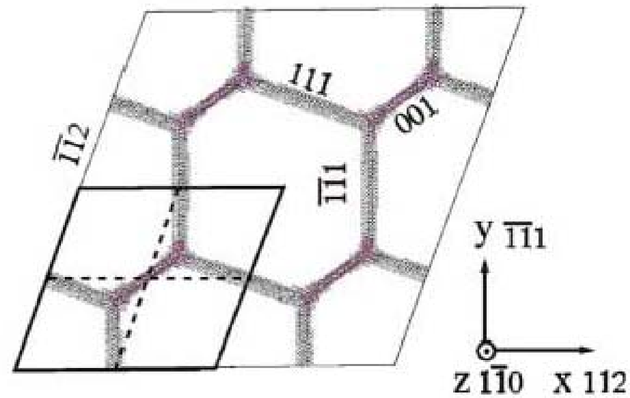
Energy-minimizing junction configuration





Atomistic simulations of Bulatov and Cai (2002)

Energy-minimizing configuration of junction, computed using line-tension approximation

Concluding remarks

- The computation of the elastic energy is greatly simplified in the dilute limit: No long-range interactions, ***line tension***!
- ***Dilute*** discrete dislocation models are well-suited for ***kMC*** implementation: Tables of segments, elementary loops, flips...
- Approach advantageous with respect to full $O(N^2)$ elastic-energy calculations, e.g., for simulations of dislocation dynamics and forest hardening
- Caveat: Not clear mathematically that line-tension approximation can be applied in the presence of ***kinetics***, ***time-evolution***…