The Dilute Limit of Discrete Dislocations: Application to Dislocation Junctions

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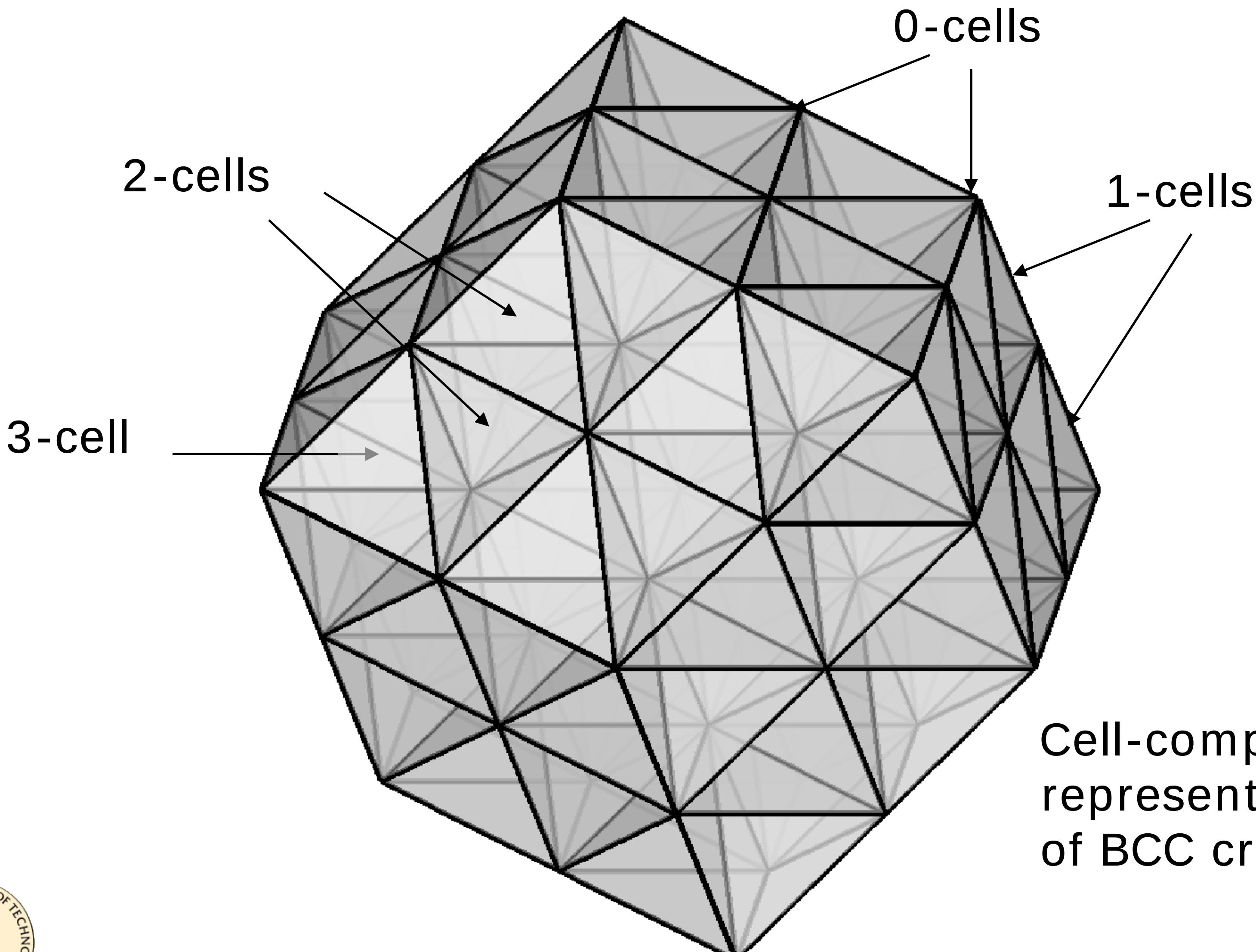
Outline

- The problem: To determine the low-energy configurations of a dislocation ensemble
- The model: Discrete dislocations on discrete lattices interacting through discrete Green's functions
- The results:
  i. *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!)*
  ii. ***Kinetic Montecarlo solver*** *based on the limiting energy*
  iii. *Application* ***dislocation junctions***

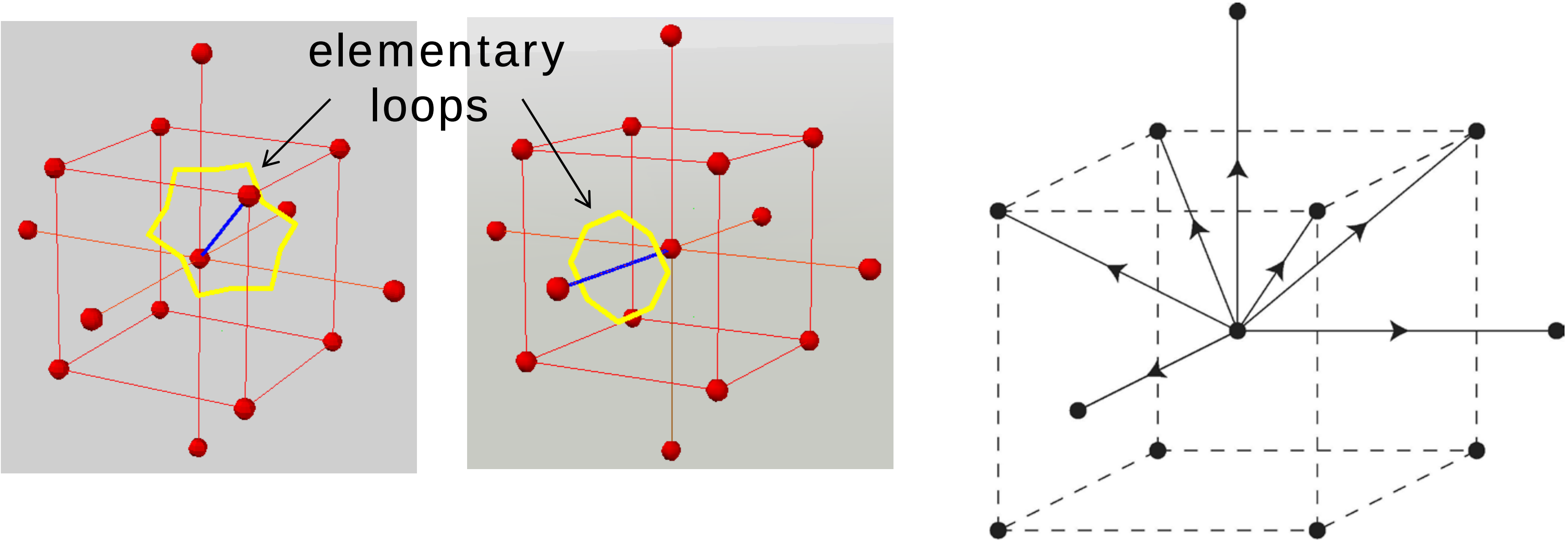
Lattice cell complexes



Cell-complex representation of BCC crystal

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

Elementary dislocation loops

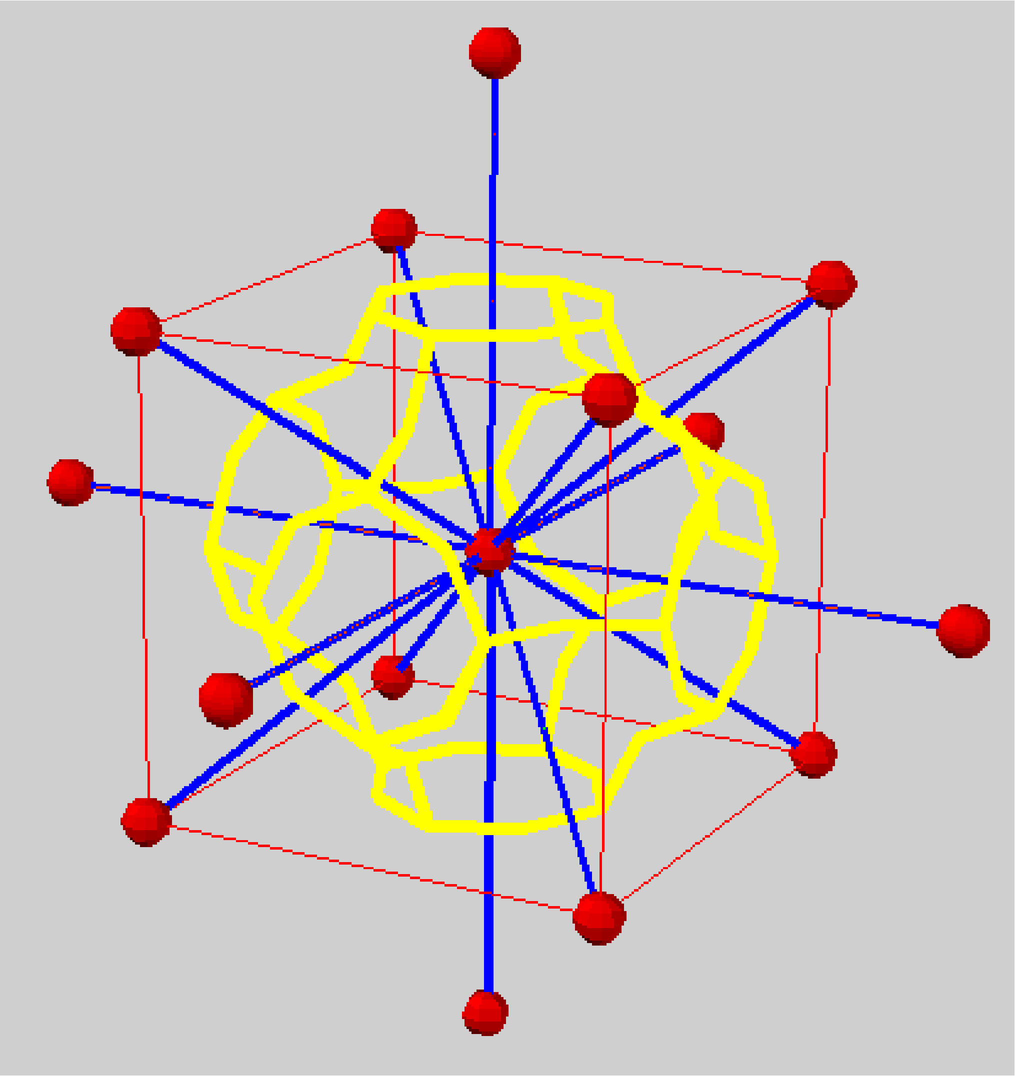


- Shown dislocation loops, their symmetry-group orbits and their translates form a basis for all closed discrete dislocation loops
- There is an elementary loop per atomic bond (1-cell) of lattice

- 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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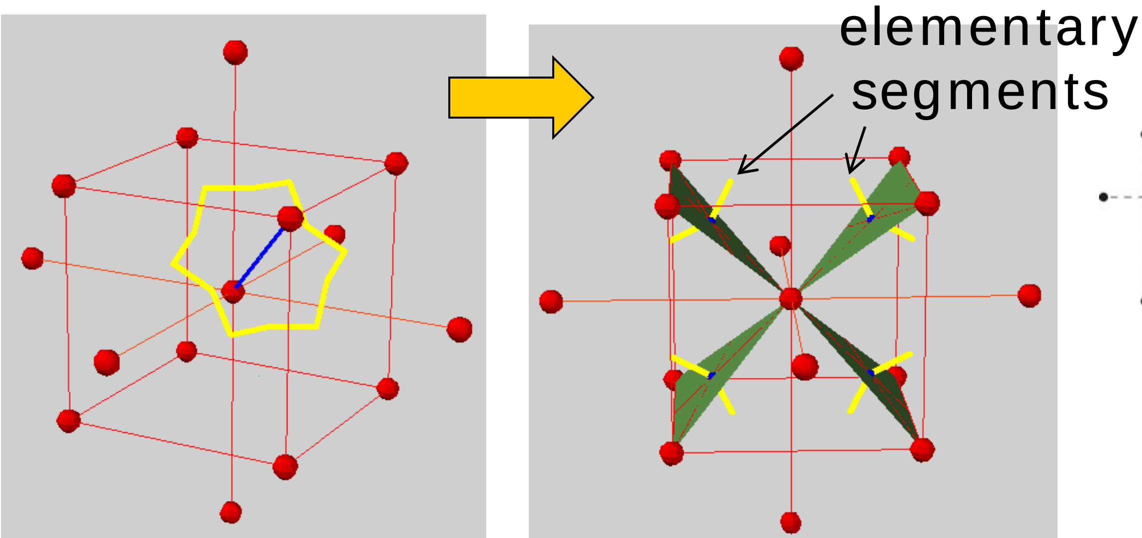
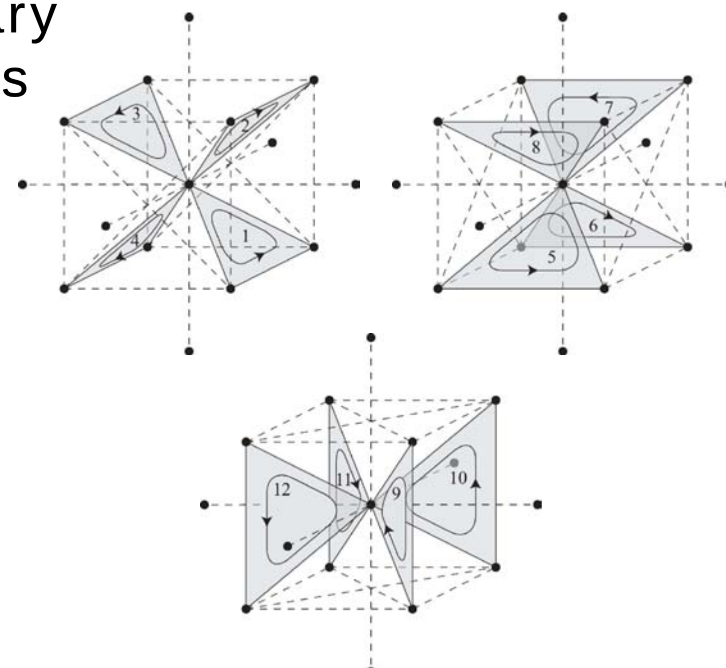
Elementary dislocation segments





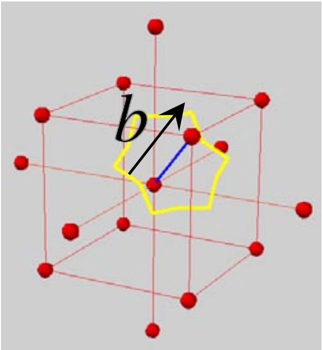
- Elementary dislocation loops can further be decomposed into elementary dislocation segments
- There is an elementary segment per face (2-cell) of lattice

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

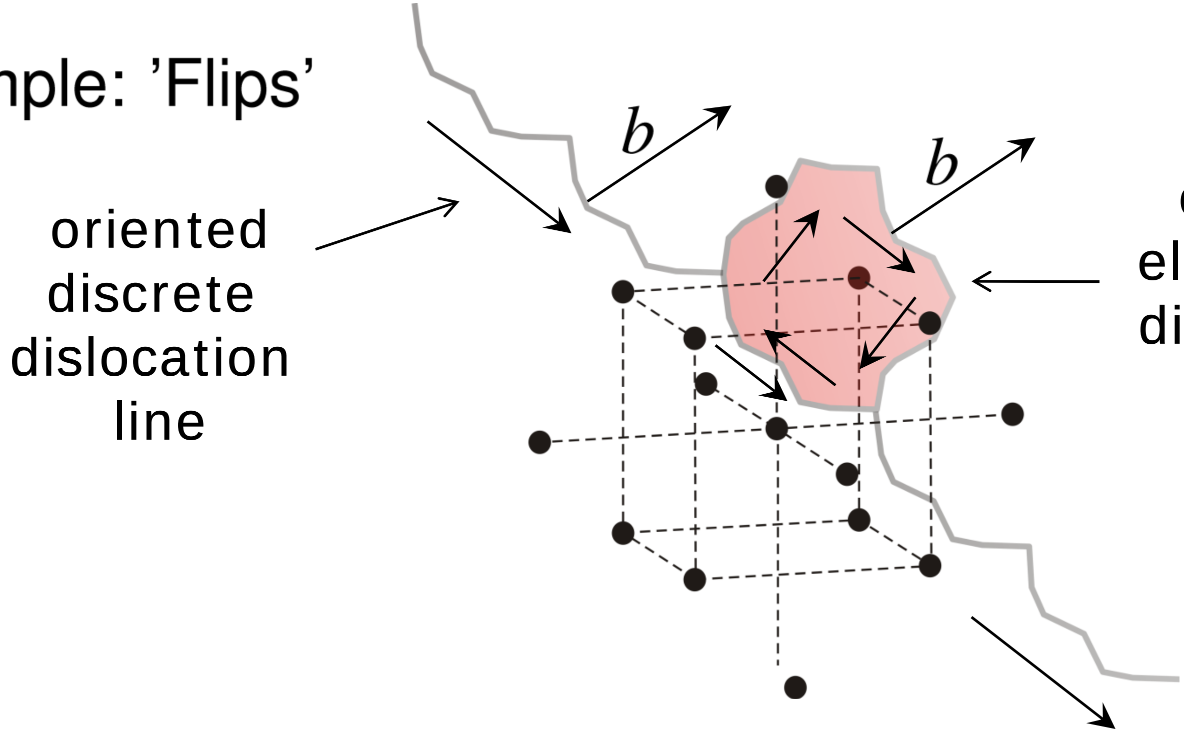
- 12 types of elementary segments!

Discrete dislocation densities

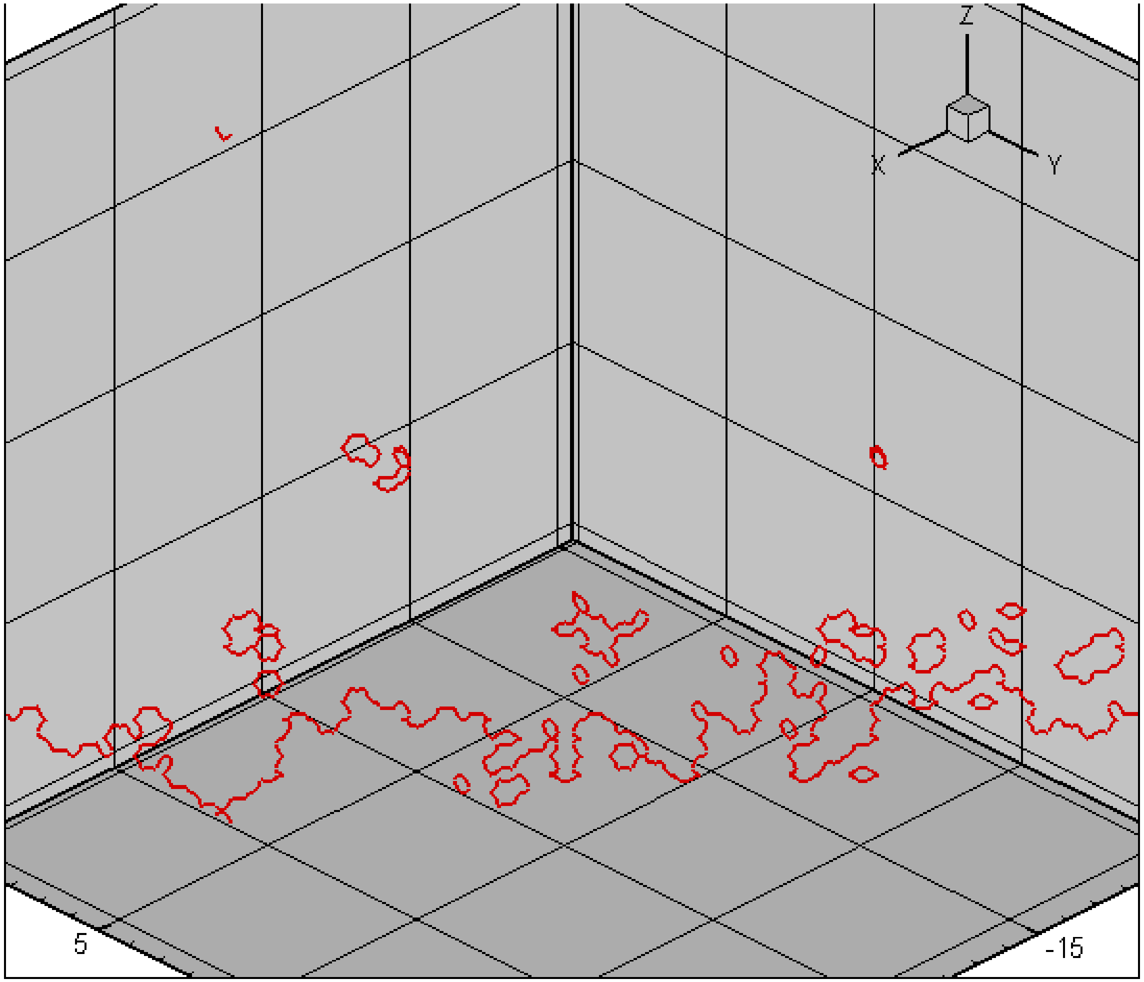
- Discrete dislocation density α:
  - Assign Burgers vectors to elementary loops
  - Add up algebraically all 'loaded' loops



- Example: 'Flips'



Discrete dislocation densities



Complex discrete dislocation line generated through a sequences of flips

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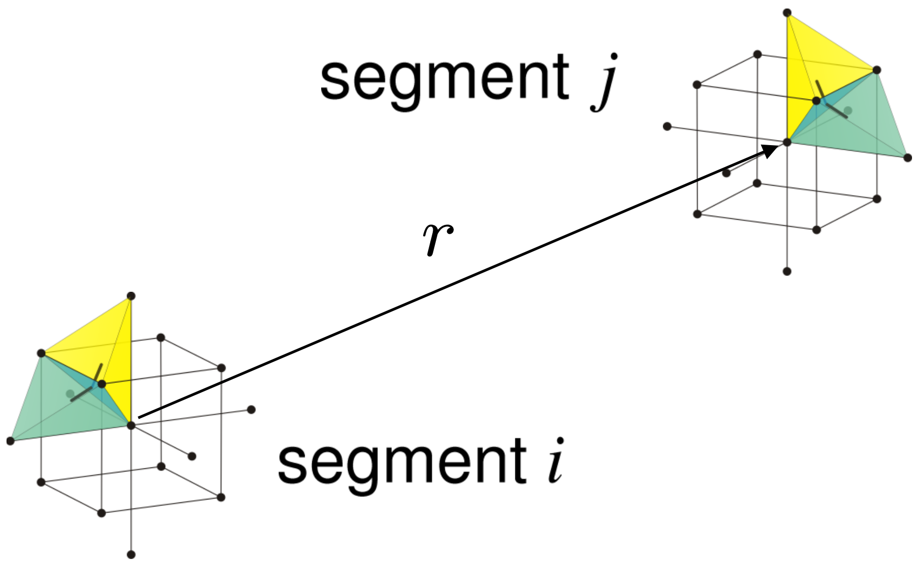
Discrete dislocations – Elastic energy

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

$\Gamma(r) \equiv$

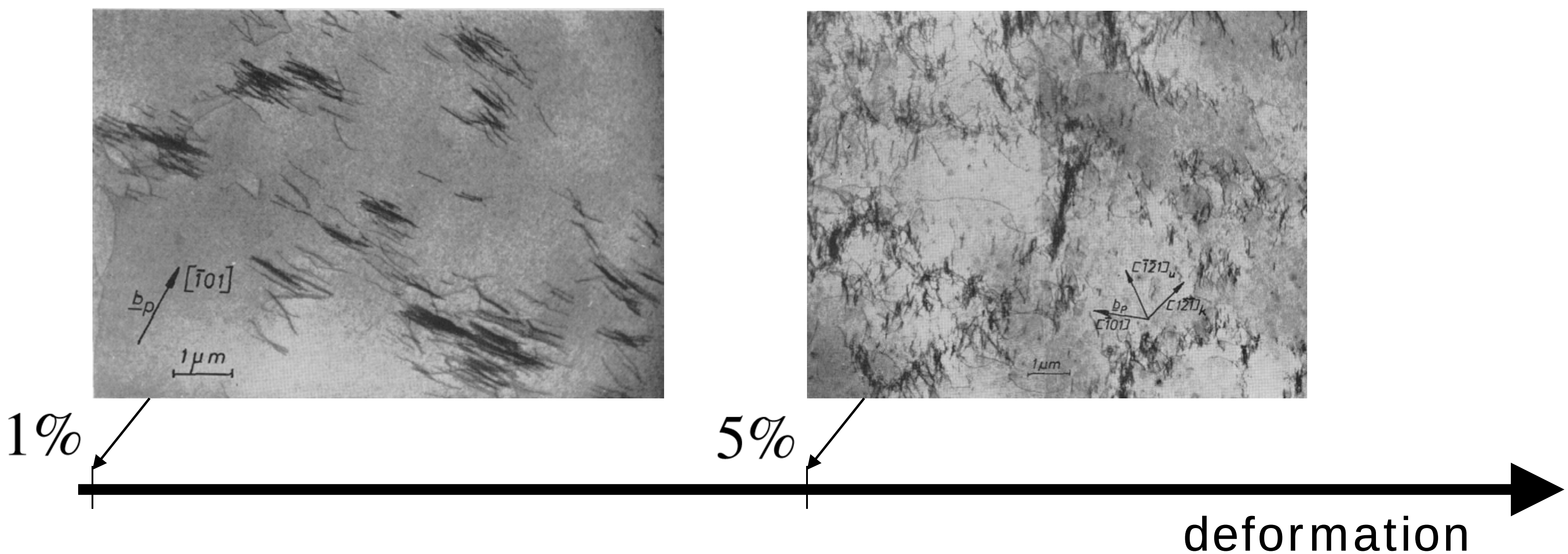


interaction energy between pair of elementary dislocation segments

- 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!

Dislocation densities are dilute

- Dislocation densities in plastically deformeed 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

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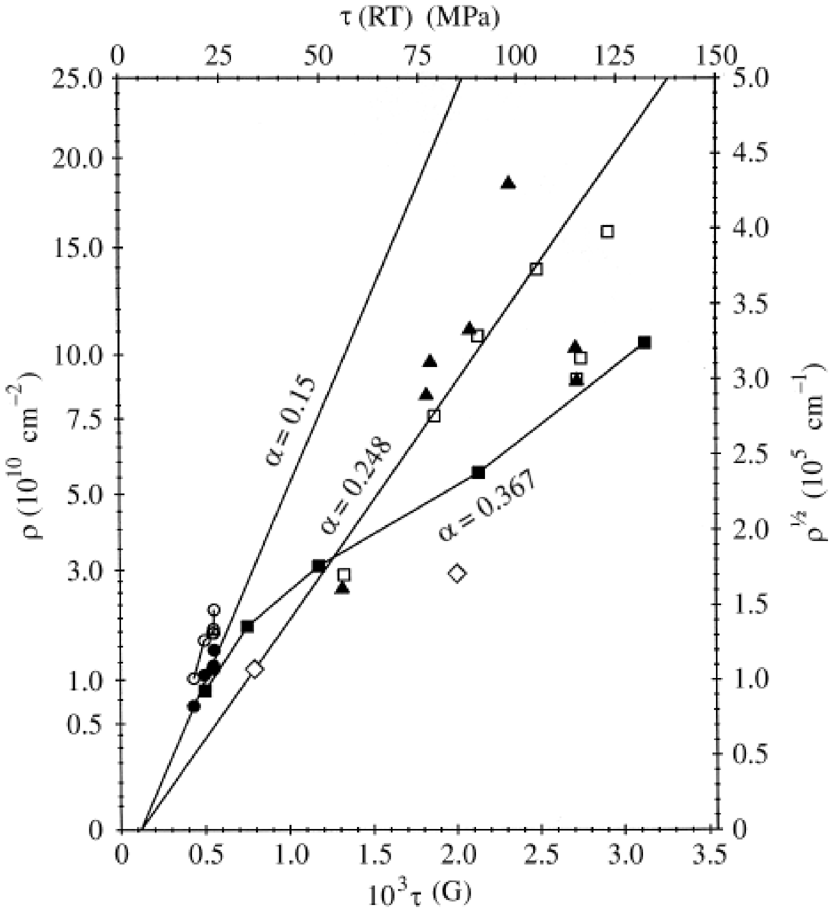
Dislocation densities are dilute

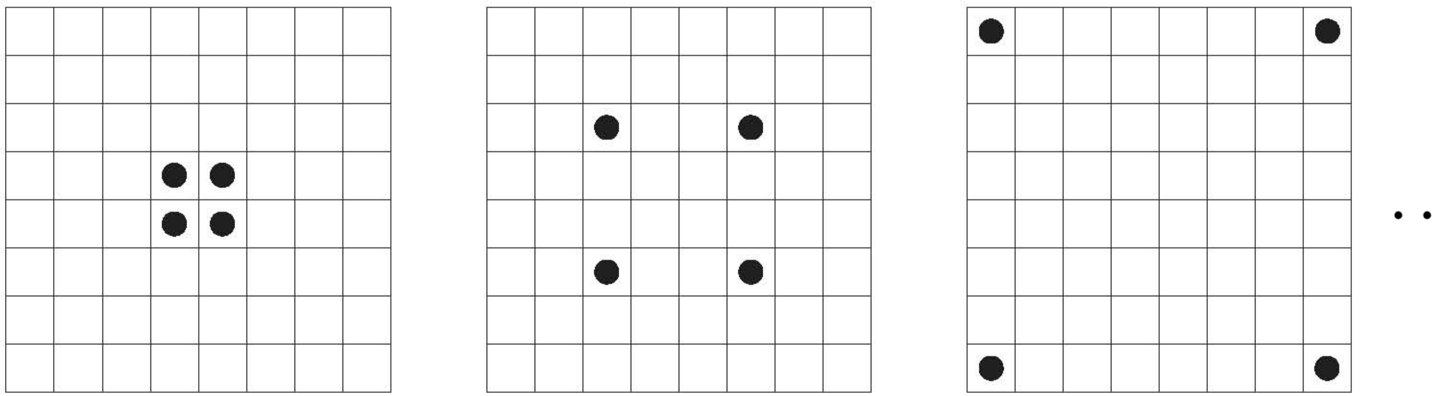


- Initial dislocation density ~ 10^{10} cm^{-2}
- Saturation dislocation density ~ 25 x 10^{10} cm^{-2}
- Initial mean distance between dislocations ~ 100 nm (278 lattice constants)
- Mean distance between dislocations at saturation ~ 20 nm (56 lattice constants)
- Investigate ***dilute limit***!

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.

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!

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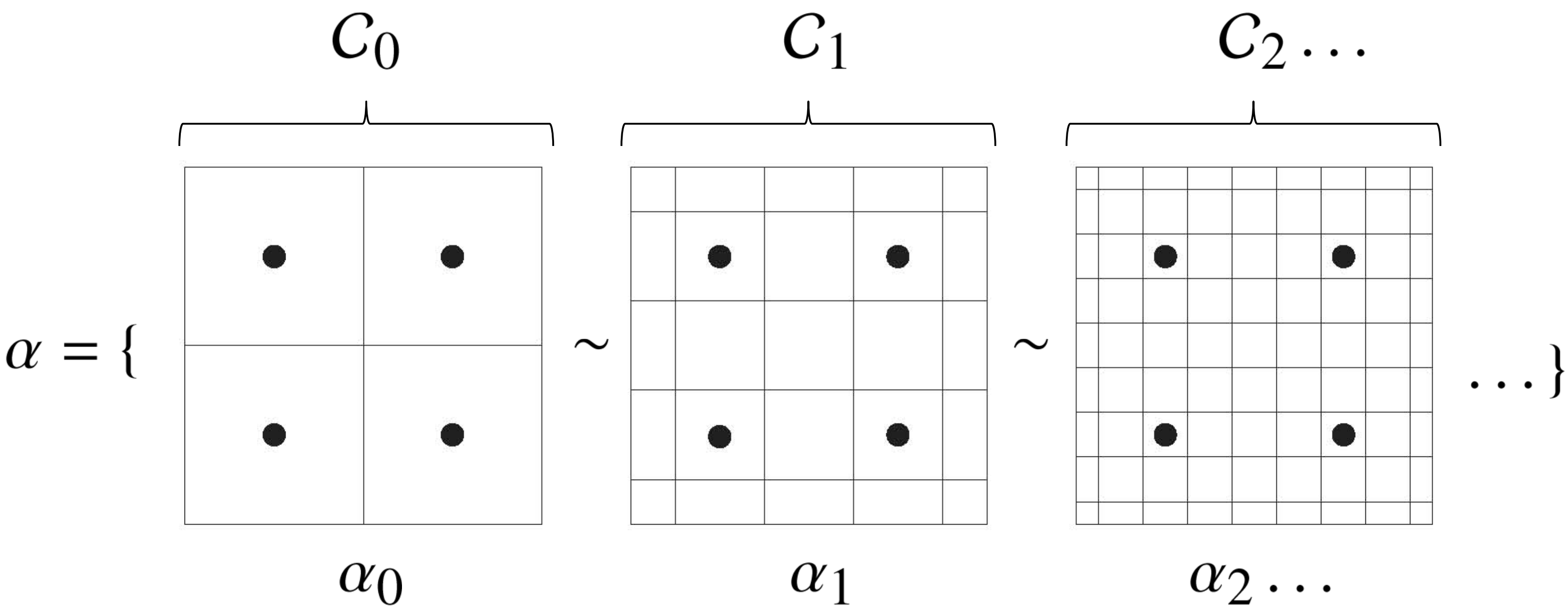
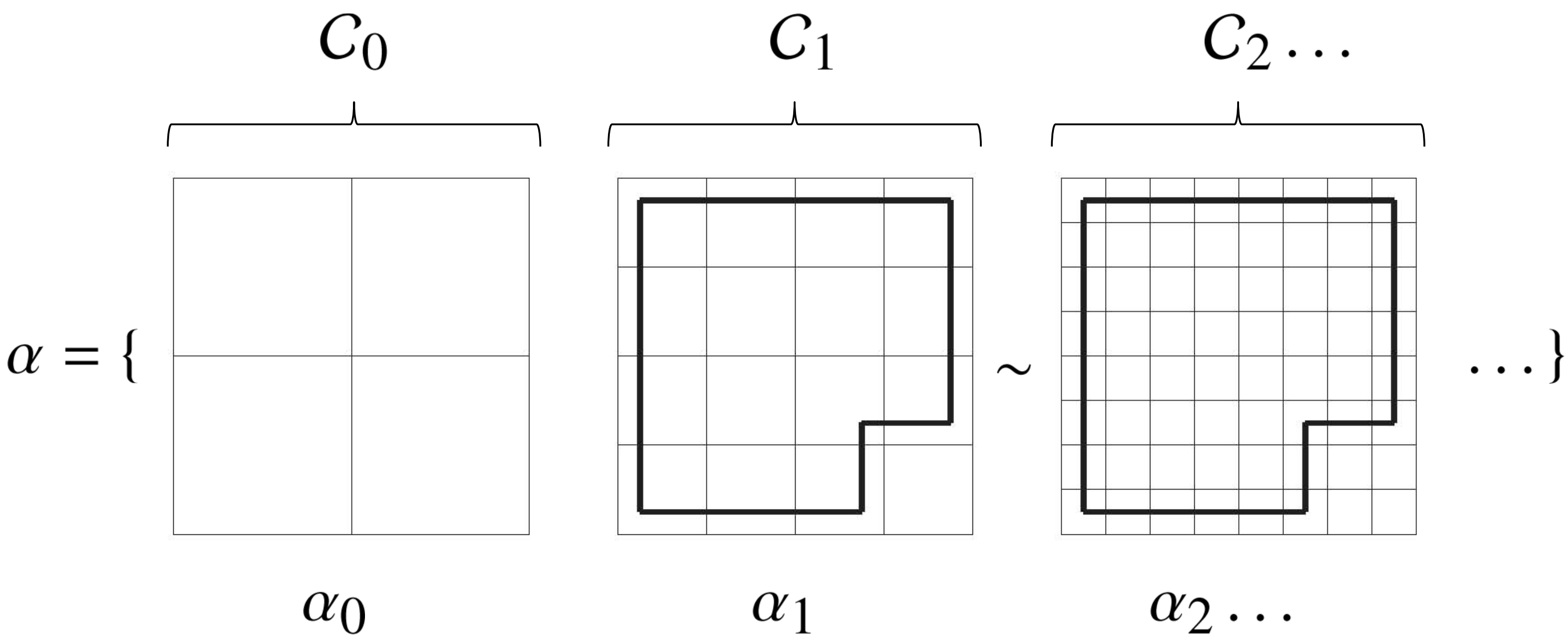
The dilute limit – Scheme II



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!
- Norm: $\|\alpha\|^2 = \sum_i |b_{hi}|^2$, independent of h

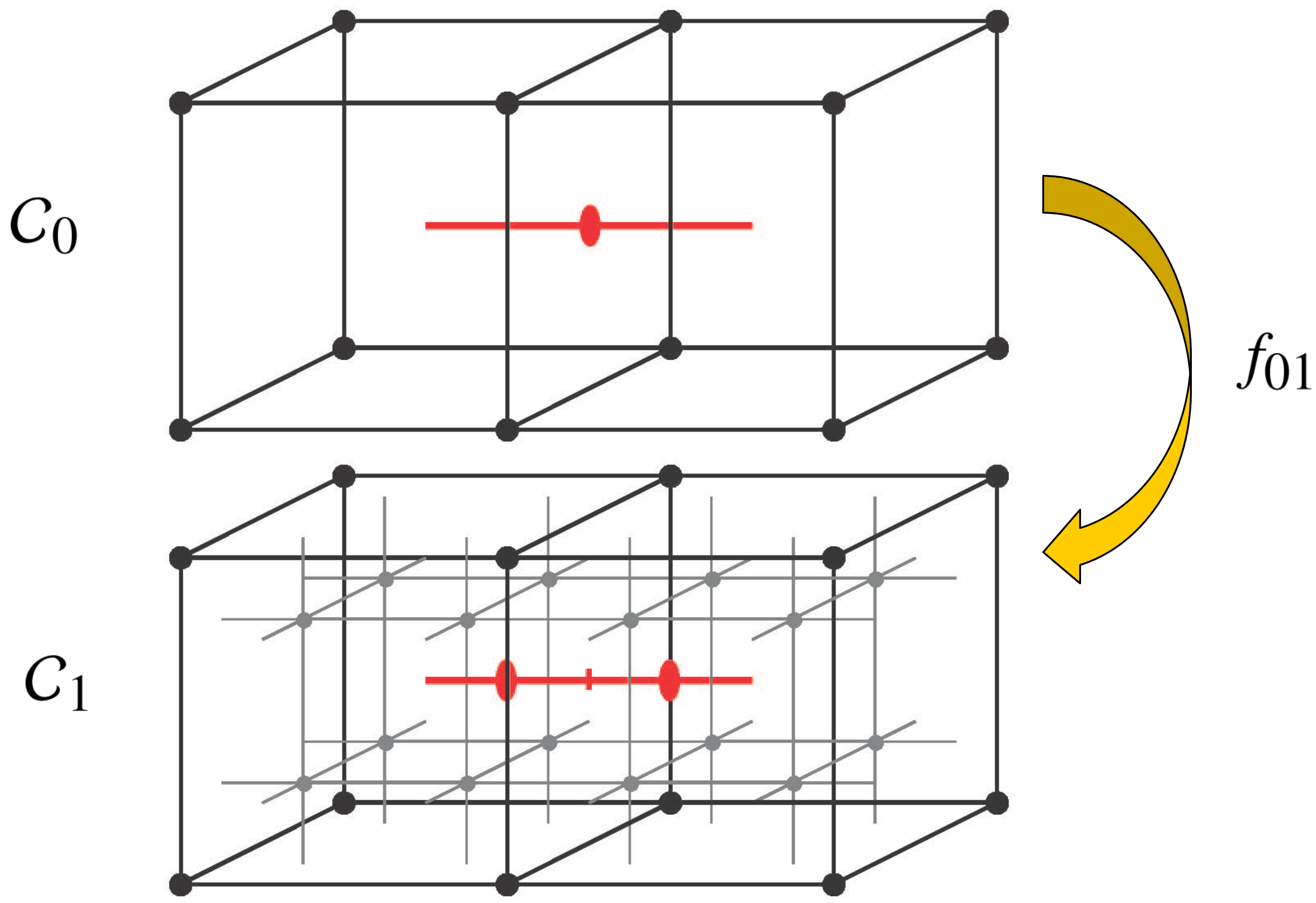
The dilute limit – Scheme II



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: $\|\alpha\|^2 = \epsilon_h \sum_i |b_{hi}|^2$, independent of h

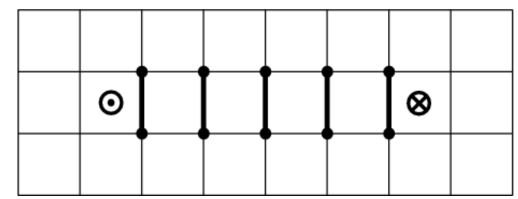
The dilute limit – Scheme II



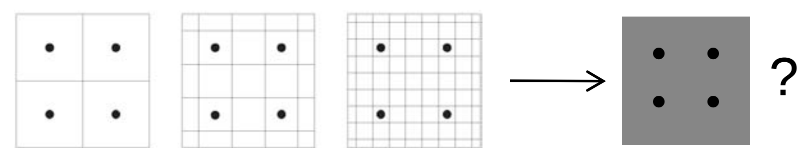
Segment refinement for cubic lattice

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, $E_h \sim \frac{\mu b^2}{2\pi} \log \epsilon_h^{-1}$



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

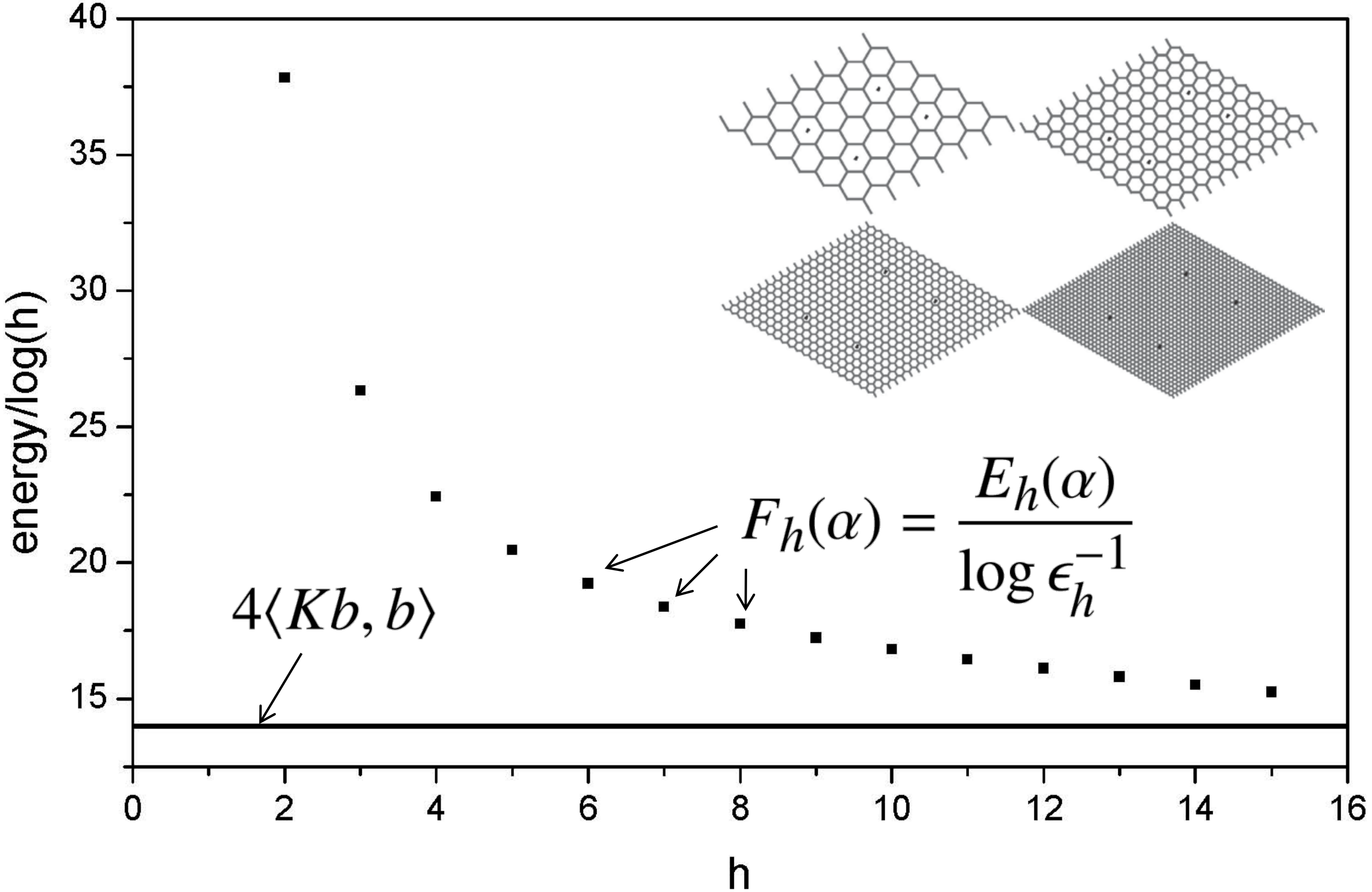


Thm $\Gamma\text{-}\lim_{h\to\infty} F_h = \sum_i \langle K b_i, b_i \rangle$ (wrt weak convergence)

$\langle K b_i, b_i \rangle$: prelogarithmic energy factor

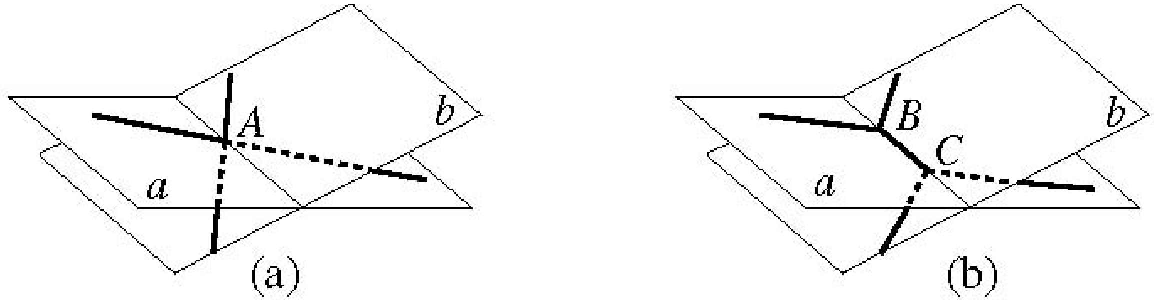
- No long-range interactions in limit $\Rightarrow$ Line tension!

Example – Graphene quadrupole

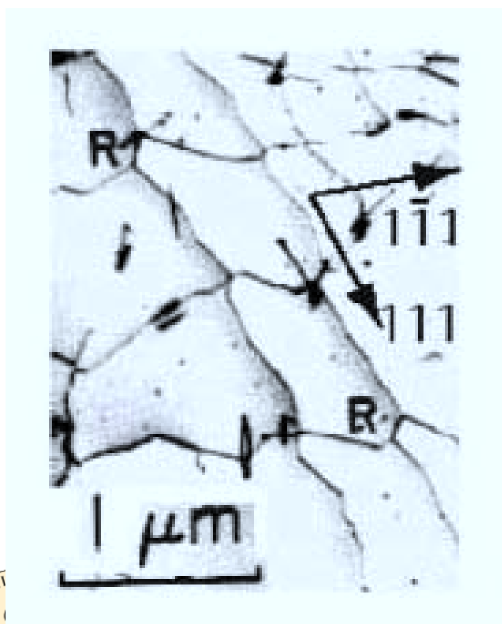


M.P. Ariza, M. Ortiz and R. Serrano,
Int. J. Fracture (2010) DOI 10.1007/s10704-010-9527-0

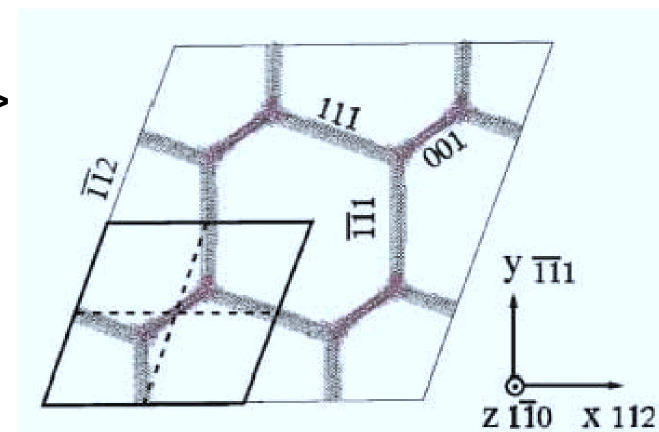
Line tension – Dislocation junctions



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



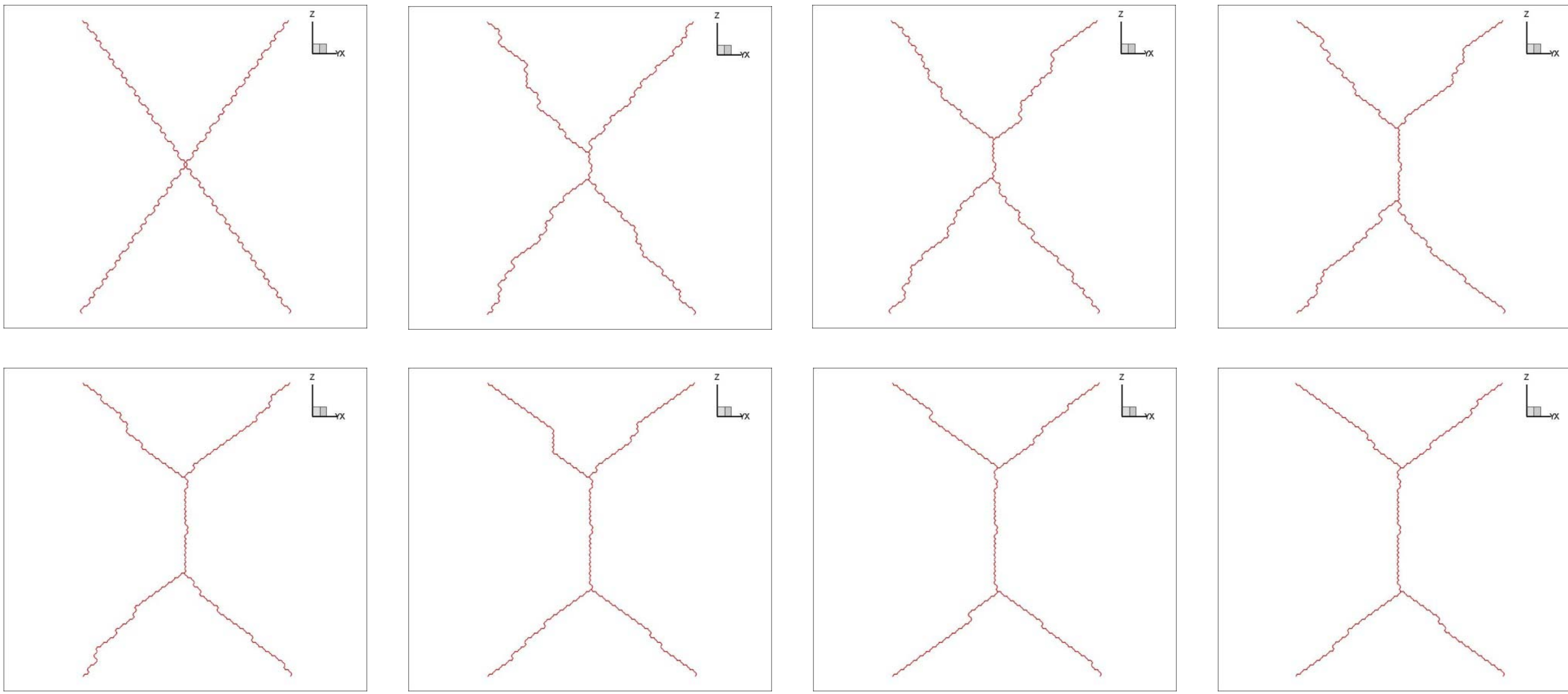
Network of ½<111> screw dislocations forming <001> screw junctions



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 .

Energy-minimizing junction configuration



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

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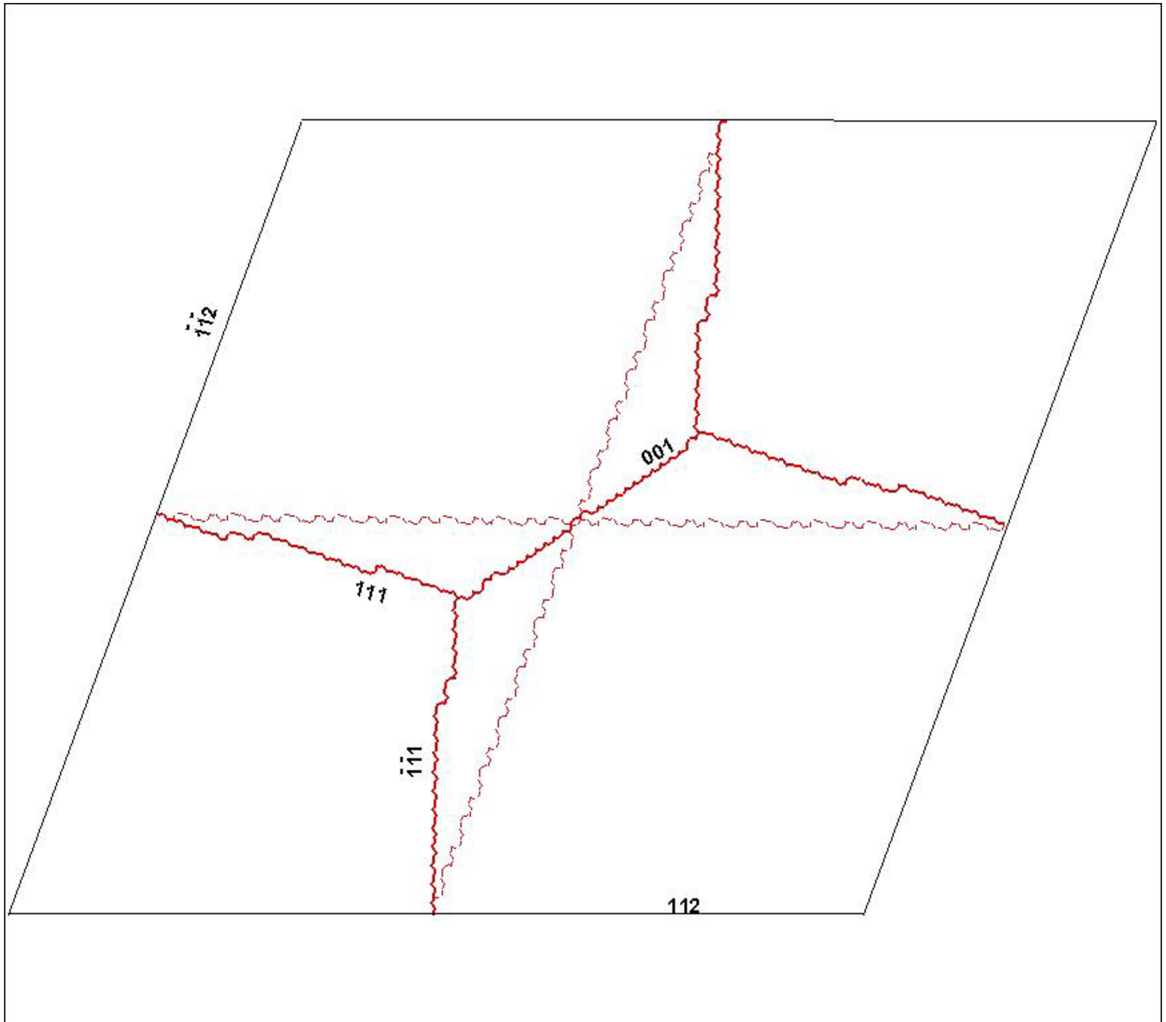
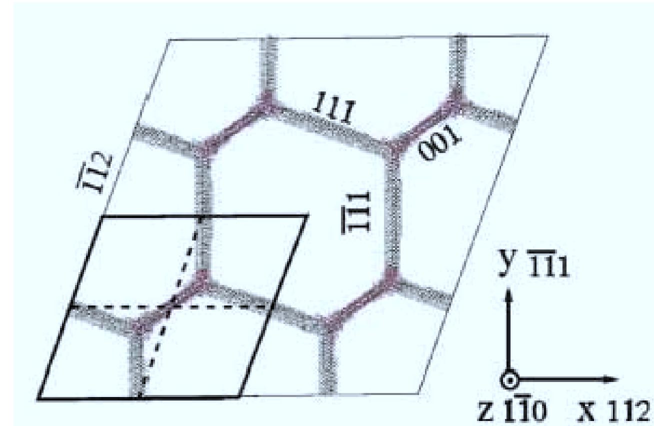
Energy-minimizing junction configuration





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 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...