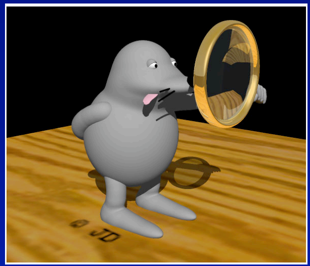

"Discrete Dislocation Plasticity"
Cambridge
Thursday 1 July - Friday 2 July, 2004

Recent progress on discrete dislocation dynamics simulations

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Outline

- A short review of DDD evolutions
- 3D-DDD
  - Piecewise line models
  - Materials specificity
    - Slip system symmetry
    - Contact reactions (junctions)
    - Velocity laws
    - Standing problems
  - Boundary Problems
    - PBC
    - Superposition or Eigenstrain methods ?
  - Computational issues
    - Fast multipole methods (Greengard)
    - Parallelization
- 2D v.s. 3D and 2.5-DDD
- Concluding remarks

Discrete Dislocation Dynamics main dates

1966	1986	1992	1998
2D inplane	2D outplane	3D (lattice)	3D (continuous)
Hardening Line tension Obstacle pinning	Patterning (1/ r)	“French touch” multi-slip	ASCI program bcc

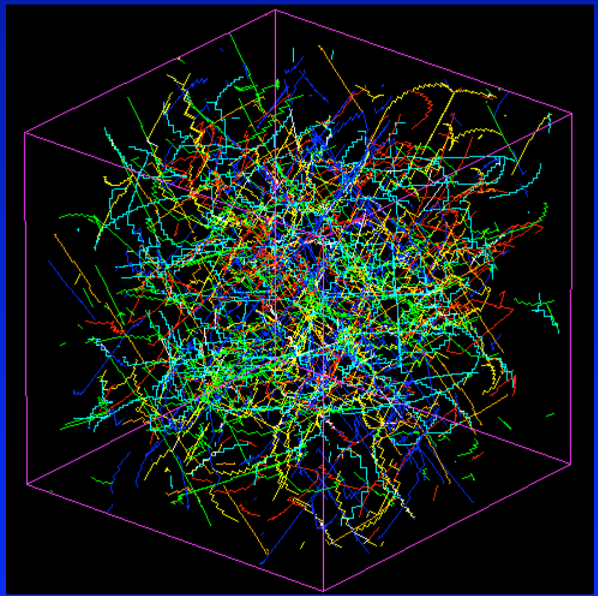
1995	1998	2001	2003
Superposition	Strong FE coupling	PBC	//
Boundary problem	Anisotropic elasticity	Mean free path	Hardening

Discrete Dislocation Dynamics (DDD)

Discretization
time & space & lines

Elastic properties
P-K force
Line tension
Loading

contact reactions
junctions



10-20 μm

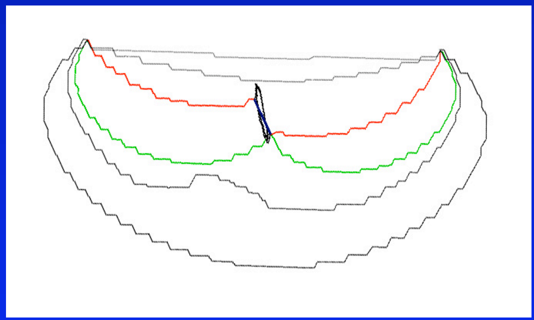
Constitutive rules
Mobility
Cross-slip

Nucleation

Boundary problem
PBC, free surface, GB, interface, etc..

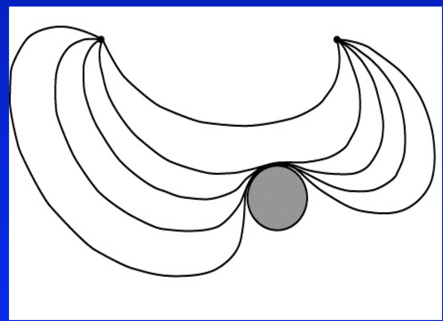
Space and line discretization

Lattice-based models



(Forest zipping-unzipping)

Quasi-continuous models

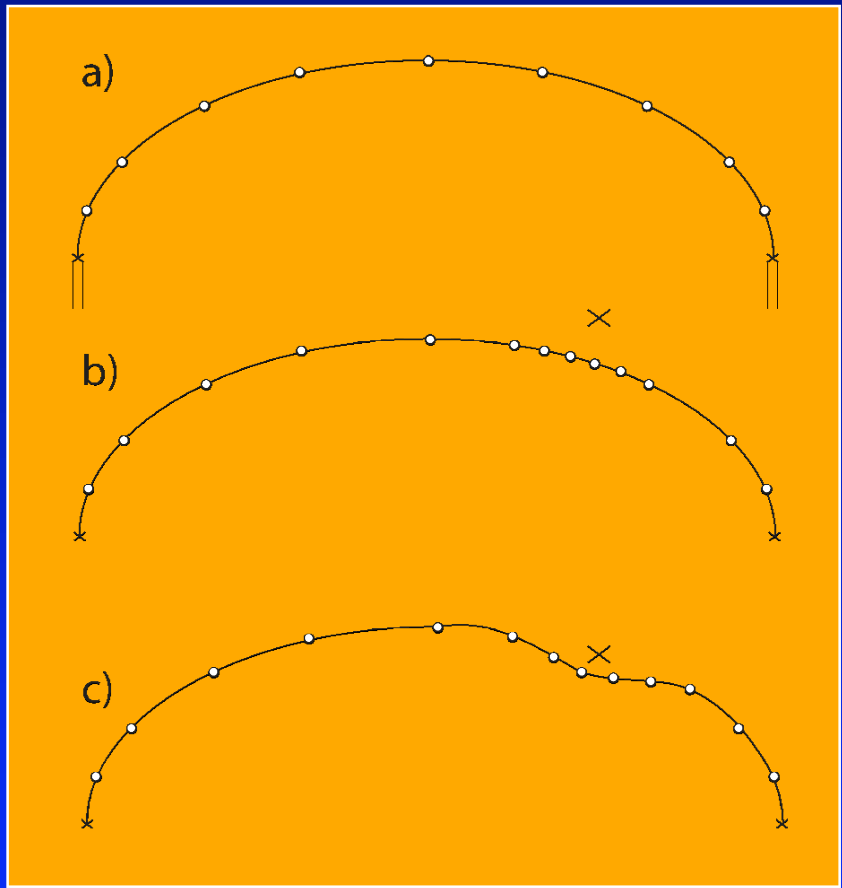


(Orowan mechanism)

Code simplicity
slip properties

Dislocation self stress field
CPU (time step ?)

Curvature v.s. elastic field gradients



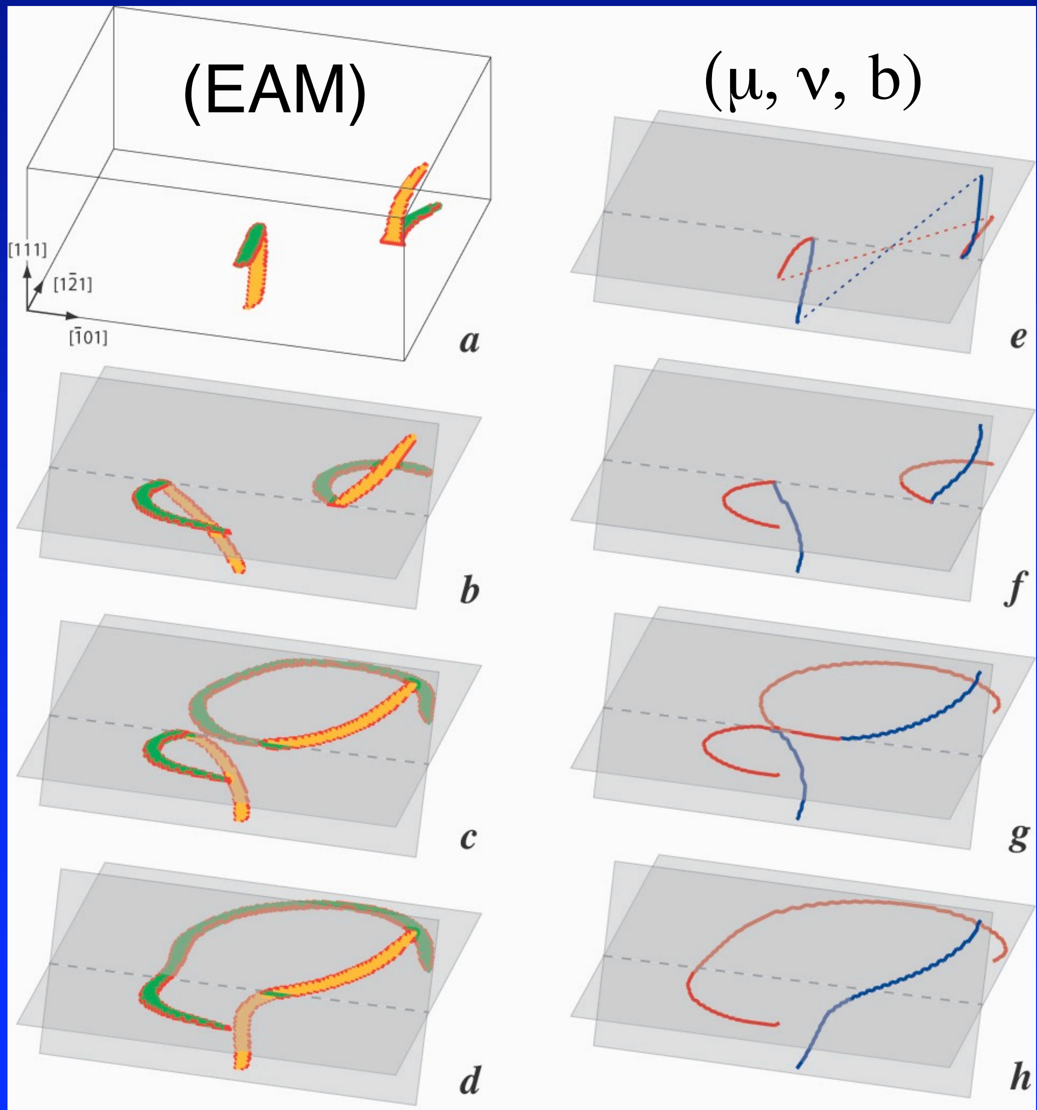
The killer is the number of integration points (IP) of the P-K force, not the number of segments needed to describe the curvature of an isolated dislocation !

How good is the elastic theory?

$\tau_c / \mu = 0$

$\tau_c / \mu = 1.85\ 10^{-2}$

Collinear annihilation



l_o=27 nm

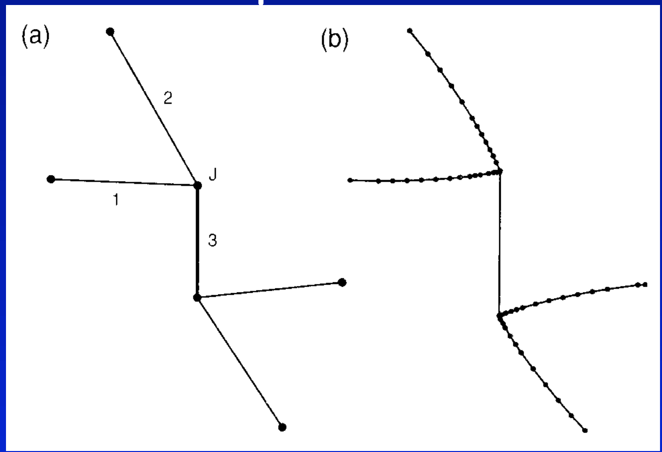
$\tau_c / \mu = 1.67\ 10^{-2}$

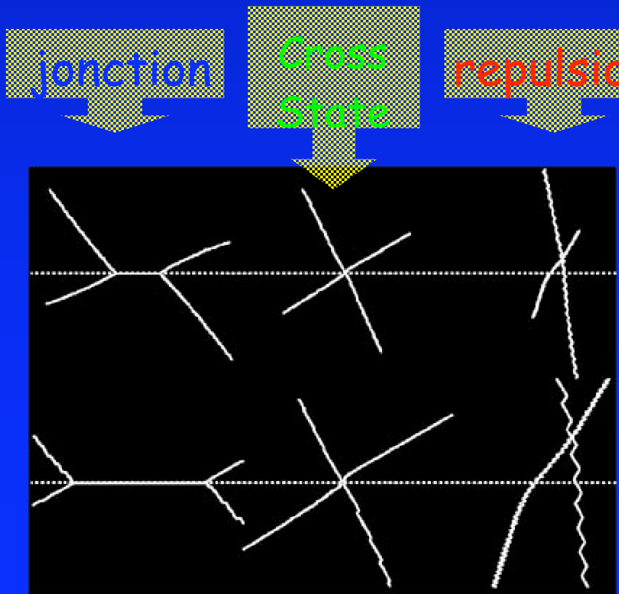
$$\tau_c = K \frac{\mu b}{l_o} Log(l_o / b)$$

Aluminium

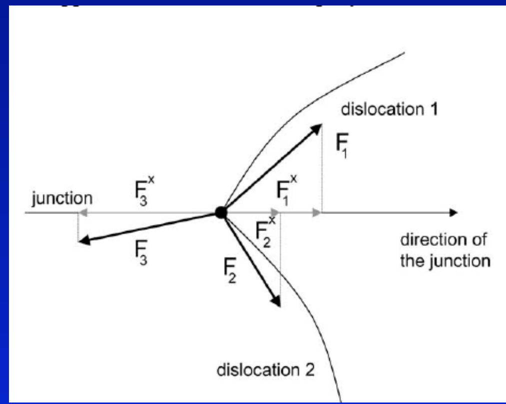
Contact reactions modeling

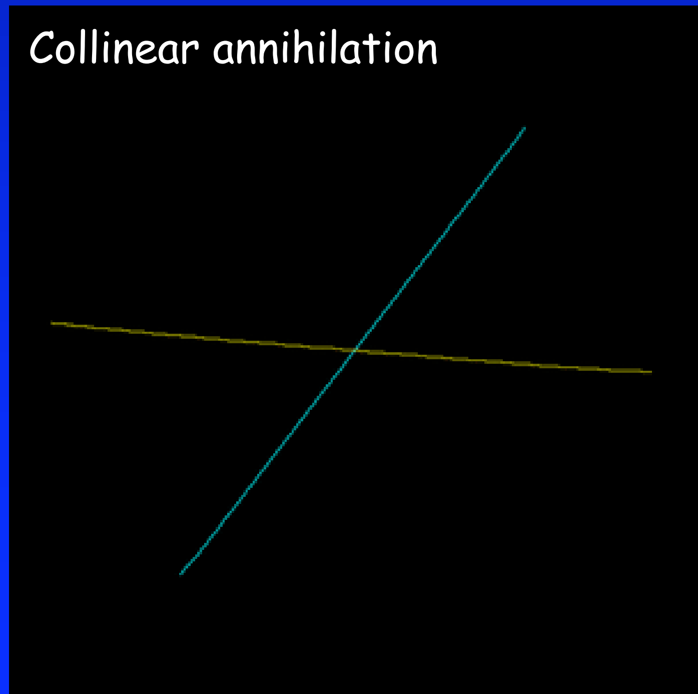
IP optimization





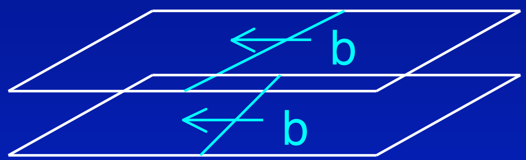
Line tension at triple nodes



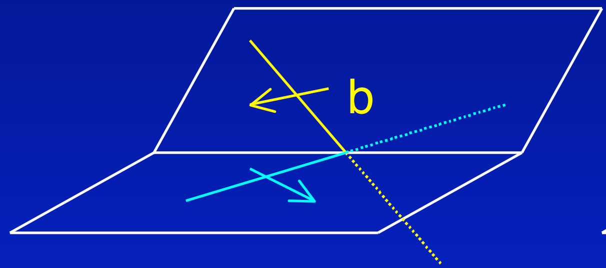


a_{ij} - Interaction coefficients - FCCs

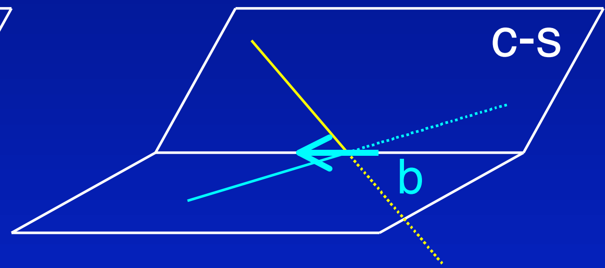
(model simulations)



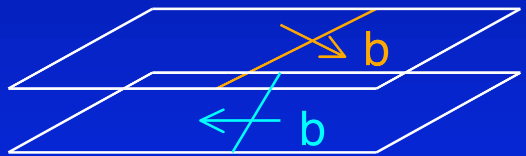
a_0: self



a_3: Lomer
a_2: glissile
a_{1ortho}: Hirth



a_{1coli}: annihilation



a_{1copla}: coplanar

Measurement: $$a^{su} = (\sigma^s / \sqrt{\sum_u \rho^u})^2$$

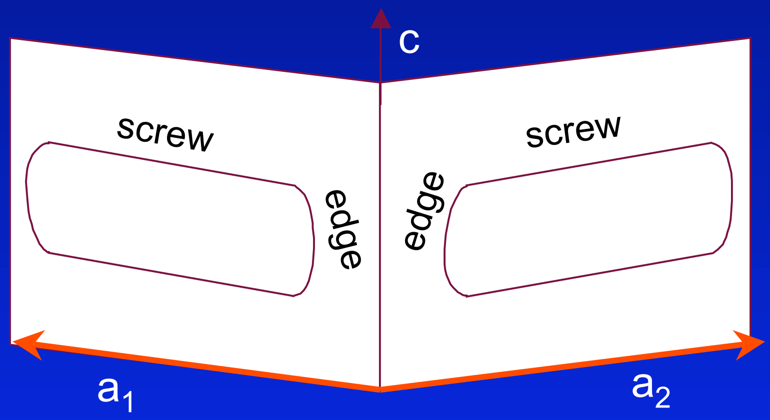
Hirth (a_{1ortho}= 0.051) Glissile (a_2= 0.075) Lomer (a_3= 0.084) a_{coli}= 1.265

Velocity laws

Viscous drag

$$v = \frac{\tau_{eff} b}{B(T)}$$

$V_{screw} << V_{non\text{-}screw}$



Lattice friction

Internal stress fluctuations!

$$v = v_o \frac{l}{l_o} \exp\left\{ -\frac{\Delta G_0}{kT} \left[1 - \left(\frac{\tau_{eff}}{\tau_0}\right)^p \right]^q \right\}$$

Segments length influence
(double kink free path)

Eg: Zirconium (prismatic)

$v_0 = 10^{14} s^{-1}$

$\Delta G_0 = 1.06$ eV : Total energy

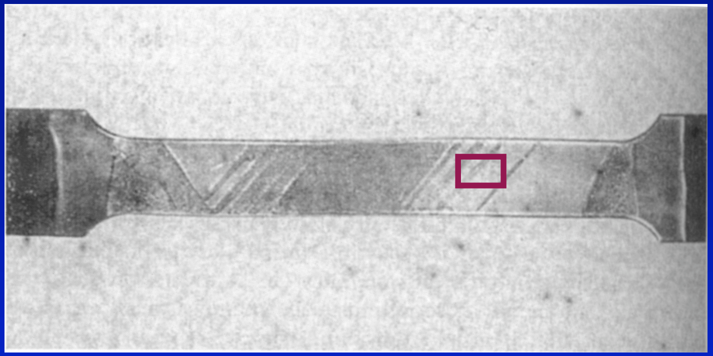
$\tau_0 = 260$ MPa : *CRSS at* 0 K

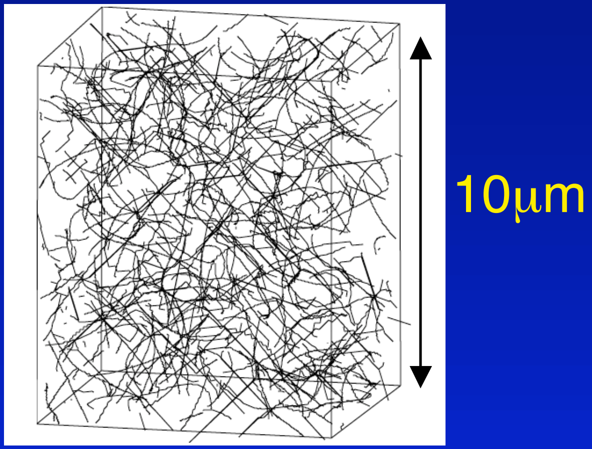
$p = 0.757, q = 1.075$

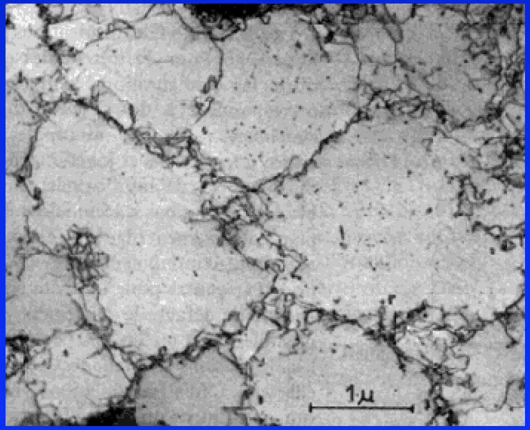
Technical standing problems in dislocation properties modeling

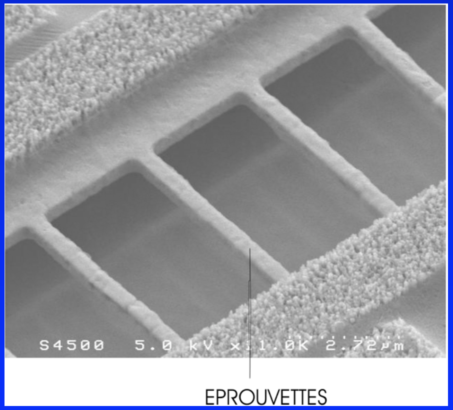
- Cross-slip in non-fccs
- Climb
- Nucleation criteria
- Transmission criteria
- Jogs and kinks in materials with lattice friction
- Over-damped motion approximation

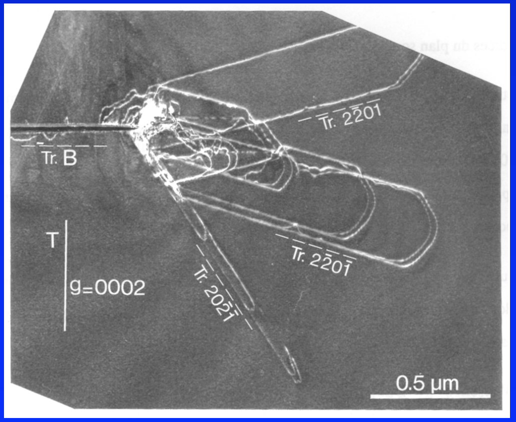
Boundary value problem





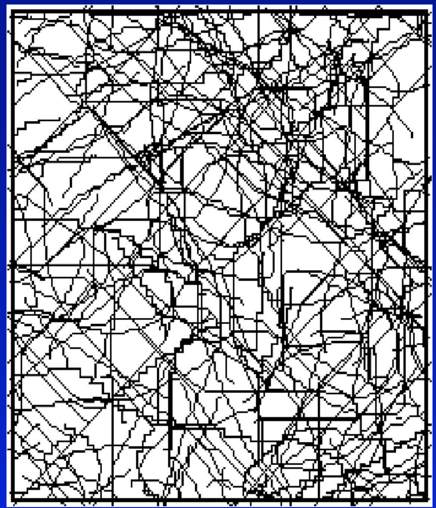






Bulk (DDD) Size effects (DDD+FE) Loading (DDD+FE)

Periodic boundary conditions

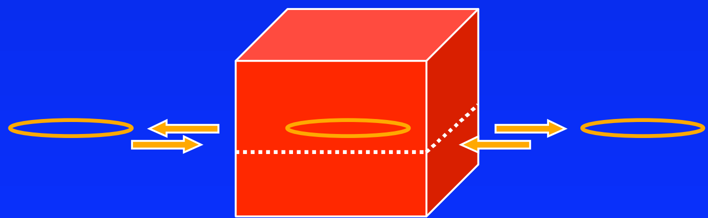


PBC

Benefits:

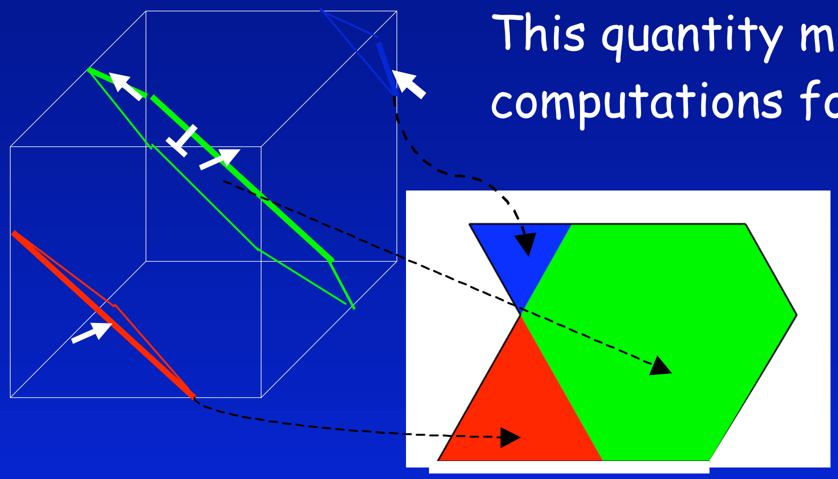
- continuity of the lines
- balance of fluxes
- internal stresses

Strong self-interactions !



- affects the density of mobile dislocations and the total dislocation storage rate.
- affects the arrangement of the microstructure and the strain hardening properties.

Dislocation mean free path



This quantity must be calculated before computations for each active slip system

(Madec, Devincre, Kubin: IUTAM 2003 proceedings, Kluwer Eds.)

(Monnet, Devincre, Kubin: Acta Mater. 2004)

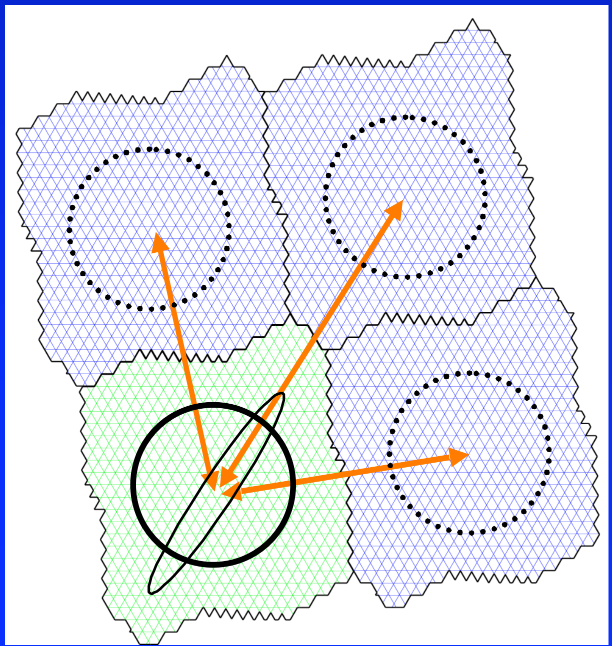
Orthorhombic box: L_x, L_y, L_z

Slip plane (h, k, l)

find 3 integers (u, v, w) such that

$$huL_x + kvL_y + lwL_z = 0$$

(first-degree Diophantine equation)



self-annihilation distance

Isotropic Loop:

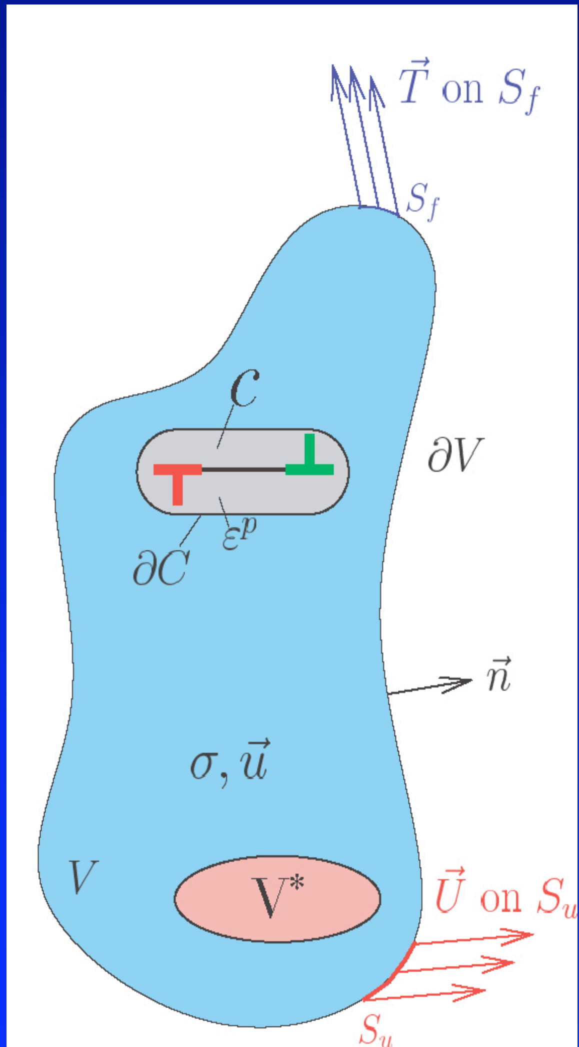
$$2\lambda = \sqrt{(uL_x)^2 + (vL_y)^2 + (wL_z)^2}$$

Anisotropic Loop:

$$\lambda = \frac{uL_x}{d_x} = \frac{vL_y}{d_y} = \frac{wL_z}{d_z}$$

with (dx,dy,dz) the fast gliding direction

Mechanical equilibrium of finite media



$$
\begin{cases}
\nabla\cdot\underline{\sigma}=0 \\
\underline{\sigma}\cdot\mathbf{n}=\mathbf{T} \text{ at } S_f \\
\mathbf{u}=\mathbf{U} \text{ at } S_u \\
\nabla\mathbf{u}=\underline{\varepsilon} \\
\underline{\sigma}=\underline{\underline{L}}^M:\left(\underline{\varepsilon}-\underline{\varepsilon}^p\right) \text{ in } V^M \\
\underline{\sigma}=\underline{\underline{L}}^*:\underline{\varepsilon} \text{ in } V^*
\end{cases}
$$

Different coupling strategies

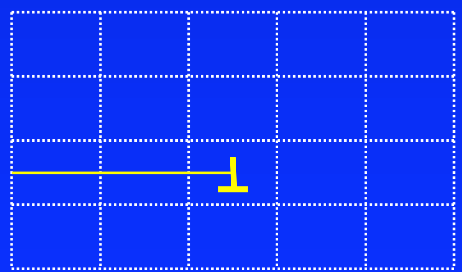
Elastic problem

FE are good to solve boundary value problems

Field singularity at dislocation cores!

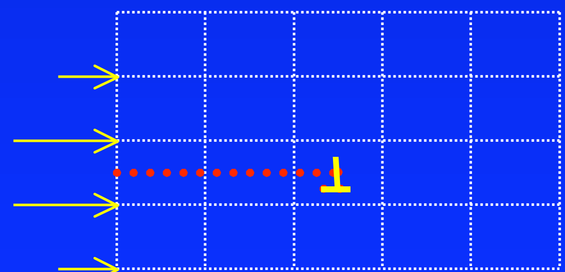
Build a FE mesh and specific procedures to capture most of the elastic fields complexity.

Eigenstrain

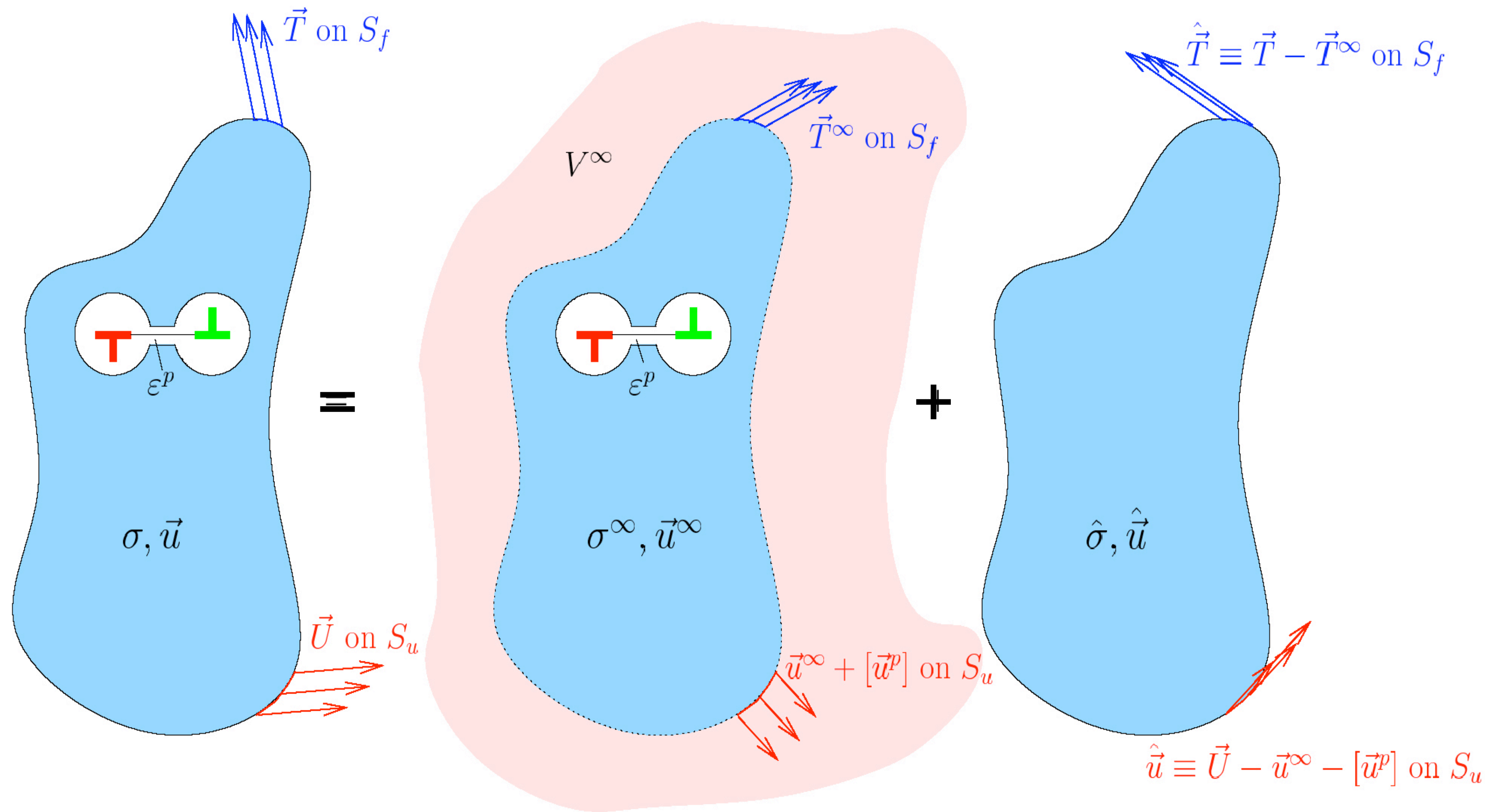


Eliminate the bulk complexity to simplify the elastic problem treated with the FE mesh.

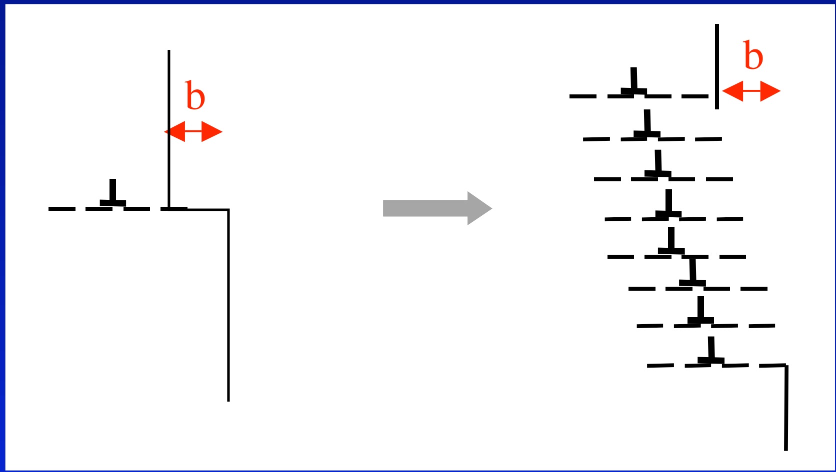
Superposition



Superposition method



Eigenstrain (homogenisation) method

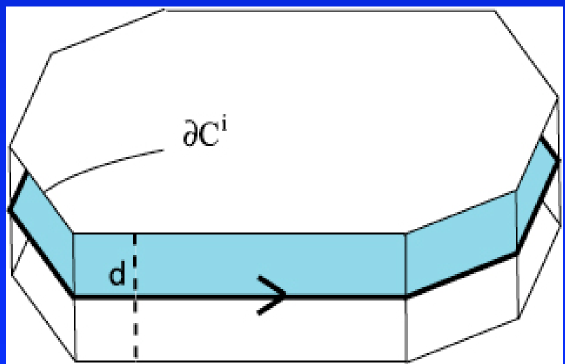


Plastic strain induced by the motion of each segment "i" at the Gauss points ",e" of the FE mesh and at time "t"

$$\Delta\gamma^i_{n,e} = \frac{\left(b^i/h\right) V^i_{\text{int},e}}{V_{G,e}}$$

$$\Delta\varepsilon^p_{,e} = \sum_i \Delta\gamma^i_{n,e}\left(l^i \otimes n^i\right)^{sym}$$

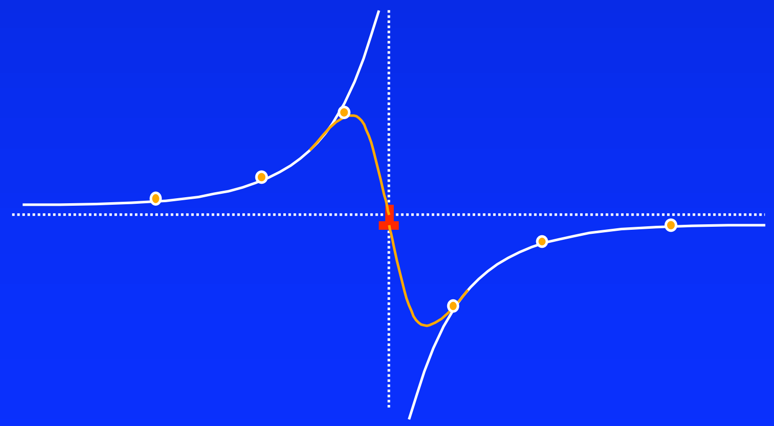
$$\varepsilon^p_{,e} = \sum_t \Delta\varepsilon^p_{,e}$$



Homogenisation slab of thickness h=1.5 $(V_{G,e})^{1/3}$ is OK with elements of 20 nodes and 27 Gauss points.

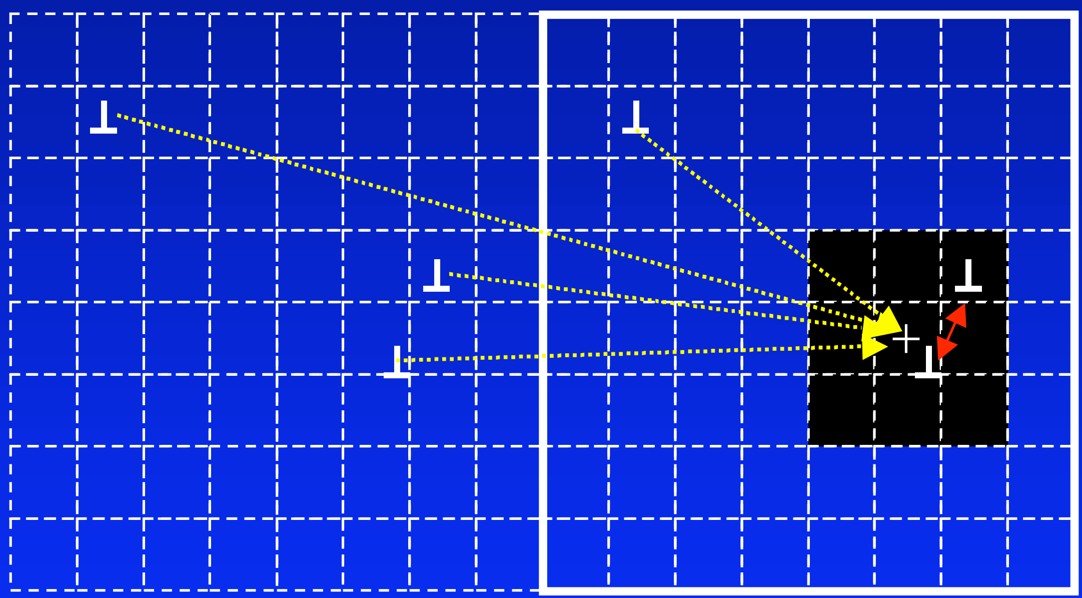
Strength and weakness of DDD-FE coupling

- Computer efficiency!
  - FE computations are faster than DDDs
- Isotropic or anisotropic elasticity !
  - Analytical forms for the displacement field
- Large deformation and surface roughness !
  - homogenisation or re-meshing
- Elastic inclusions !
- Interpolation and shape functions!



Fast multipole method
$O(N^2)$ to $O(N\log N)$ or $O(N)$

Mean field approximation: >O(NlogN)



Finite series calculation: ***O(NlogN) or O(N)***

! The number of moments needed to approximate the dislocation self-stress field is very large !

Parallel DDD codes

The LLNL battlefield :-)

Size of dislocation patterns approx 1μm

Simulation box L=10μm

Dislocation density $\rho=10^{12}m^{-2}$

Length of dislocation line $\Gamma=\rho L^3=10^{-3}$m

Discretization length d=10 nm

Number of segments $N=\Gamma/d=10^5$

One processor can only handle efficiently 10^3-10^4 segments

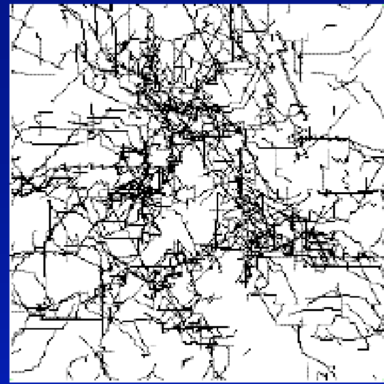
2D versus 3D

2D codes		3D codes
Easier	→	Quantitative
higher ε available		More complicated to develop
Qualitative	←	Only small strains

•2D simulations are quite rough but they can be helpful to overcome partially the numerical limitations of the 3D computations.

•On the other hand, 3D codes can be used to evaluate, in a realistic way, the dislocation mechanisms which cannot be reproduced by a 2D system (multiplication, cross-slip, pinning mechanisms strength...)

Dislocation patterning in double slip



(3D-DDD)

2.5 DDD simulation

Multiplication $\frac{\Delta\rho^s}{\Delta t} = M\dot{\gamma}^s + \text{Sources}$ $M = 2.10^{15}$

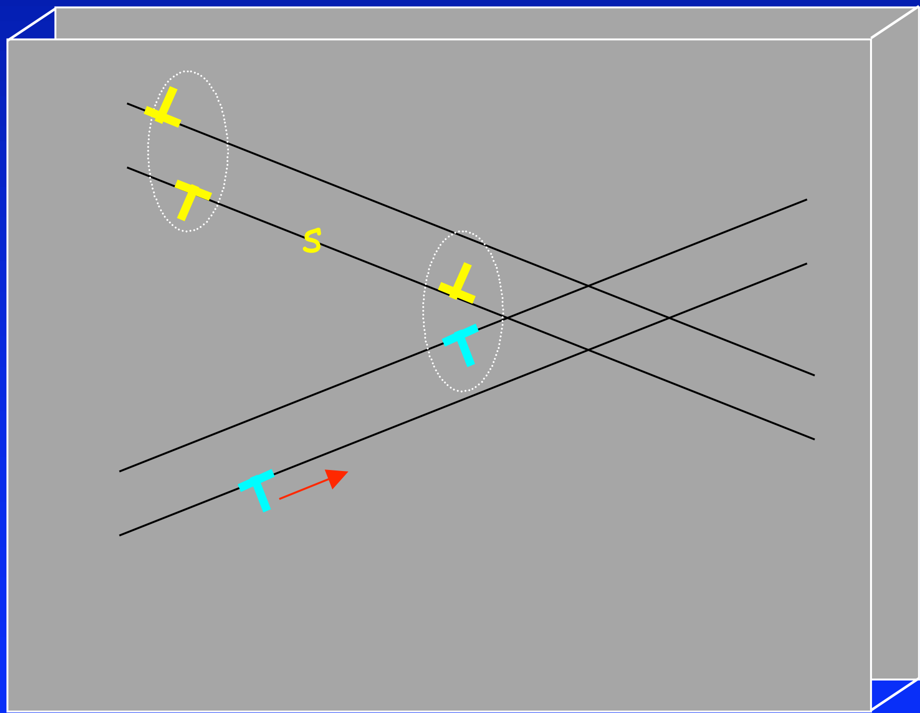
Reactions

Dipoles

Junctions

$\tau_j = \beta T = \beta \frac{\mu b}{\rho_{local}^{-1/2}} \ln\left(\frac{\rho_{local}^{-1/2}}{b}\right)$

$\beta = 0.046$



Interaction

Annihilation

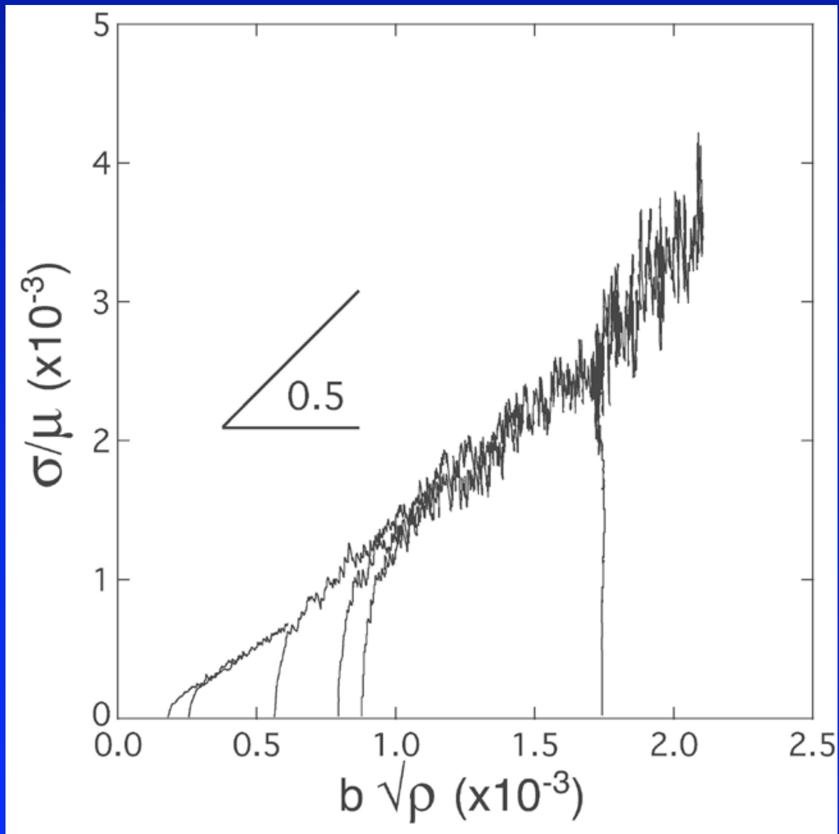
homogenization
(cross-slip)

Velocity $\left(\tau^{\text{int}}, \tau^{app}, T\right)$

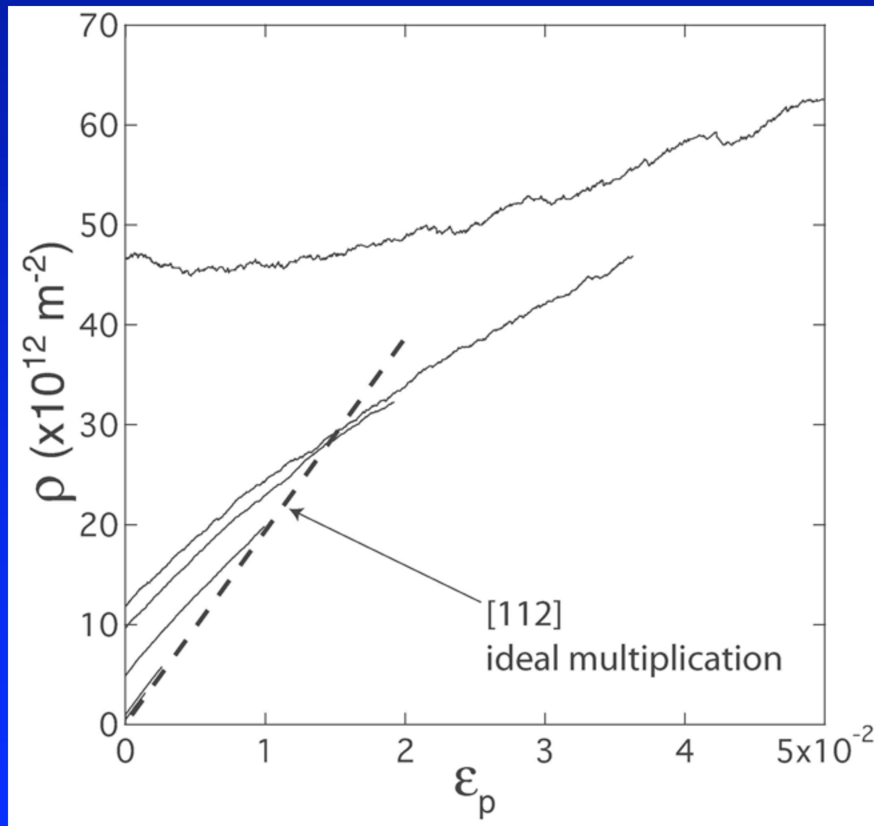
Forest model and Strain hardening

$$h = \frac{d\sigma}{d\varepsilon} = \frac{d\sigma}{d\rho}\frac{d\rho}{d\varepsilon}$$

flow stress - junction strengthening



multiplication rate - recovery

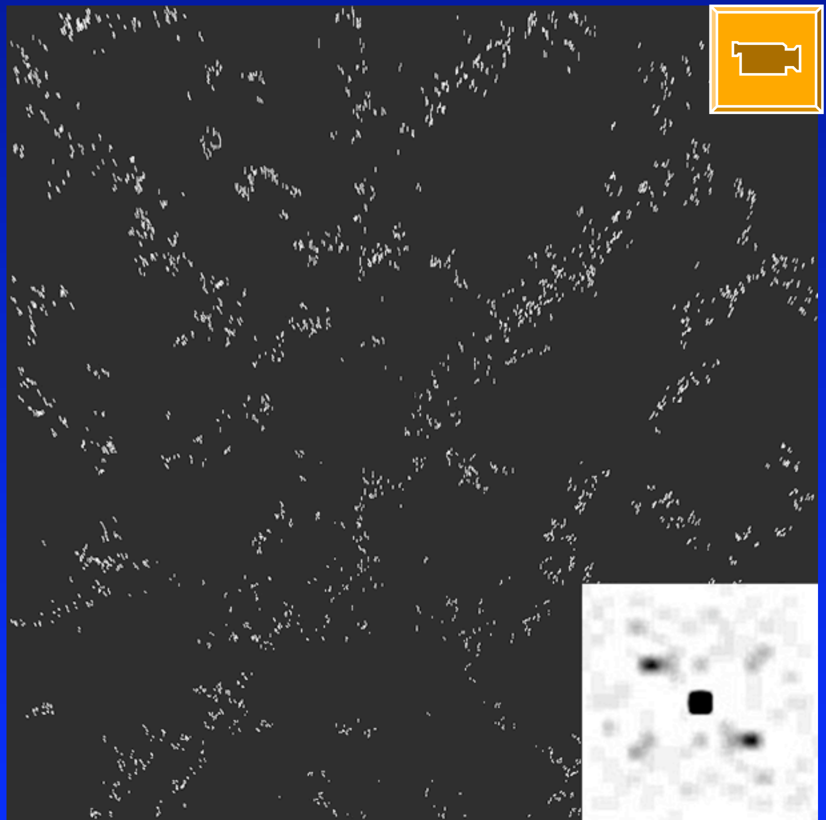


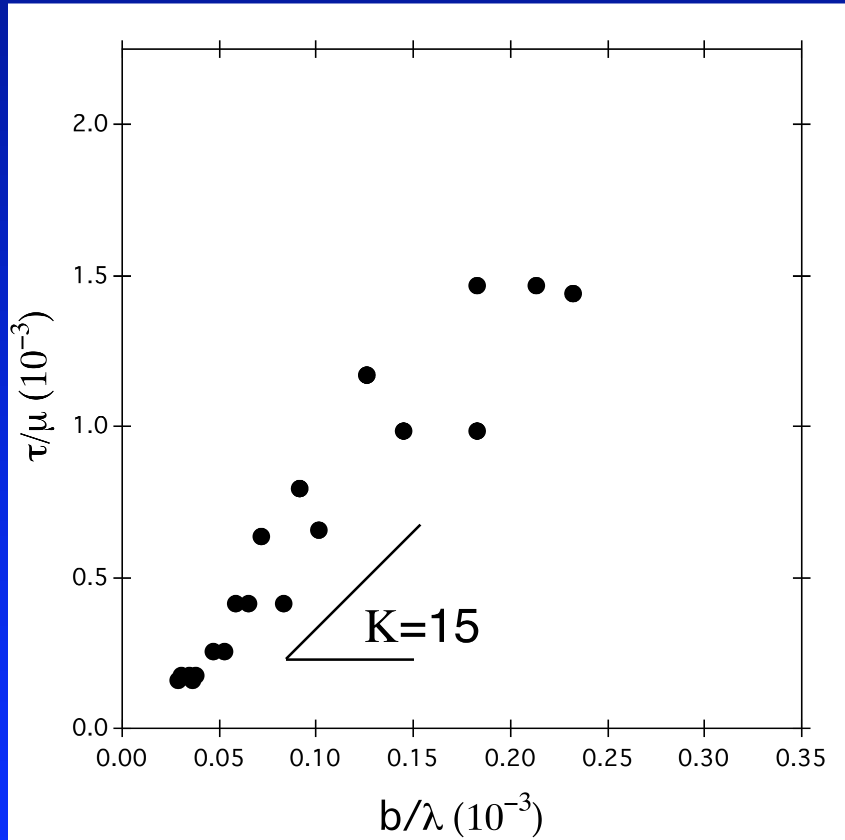
Dislocations patterning

Self-organization

Similitude principle

$$\frac{\sigma}{\mu} = K\frac{b}{\lambda}$$





Fluctuations of the long range interaction are not essential

Concluding remarks

- The elastic theory of dislocations is powerful
- Material specificities are coming up from the core properties
- PBC are useful, but dangerous
- Solving boundary value problems in 3D is a tough job, still in progress.
- Thanks to multipole algorithm and // codes, larger plastic strains should be available in the near future.
- Need for a rigorous validation and intercomparison of the various approaches currently utilized.