Microstructure Mechanics
Dislocation dynamics

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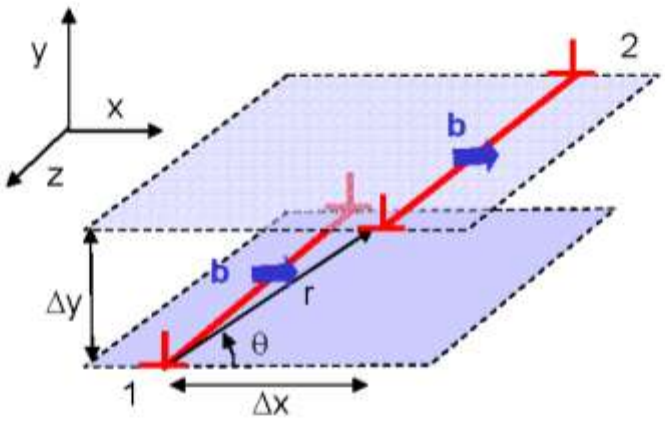


Dislocation 2 "feels" the stress field of dislocation 1 (and vice versa).

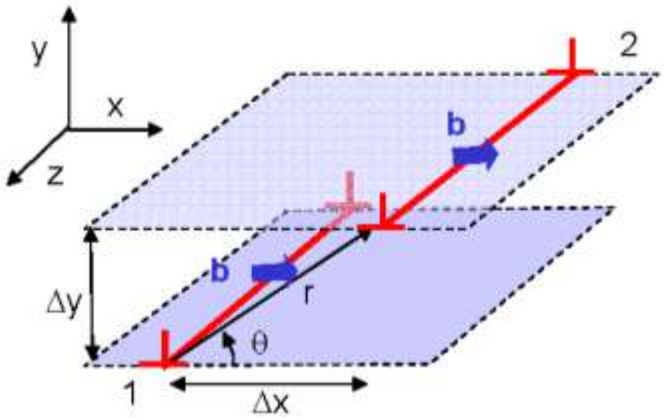
Peach-Koehler Force

$$\vec{F}_{1\to2} = \left(\underline{\underline{\sigma}}^{1\to2}\,\vec{b}_2\right)\times\vec{t}_2$$

$\boldsymbol{\sigma_{xy}}$ – produces *glide* force

$\boldsymbol{\sigma_{xx}}$ – produces *climb* force

Forces among edge dislocations

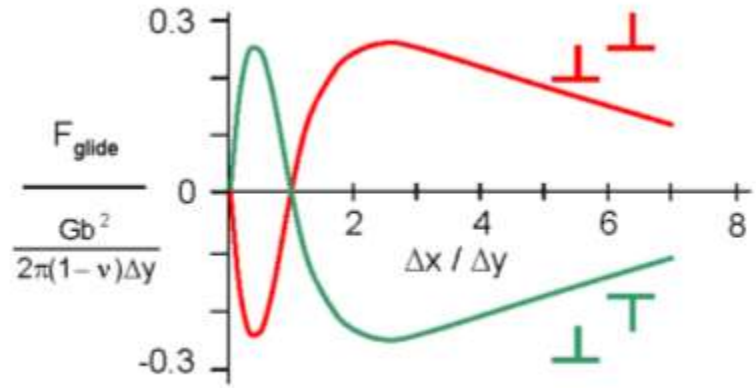


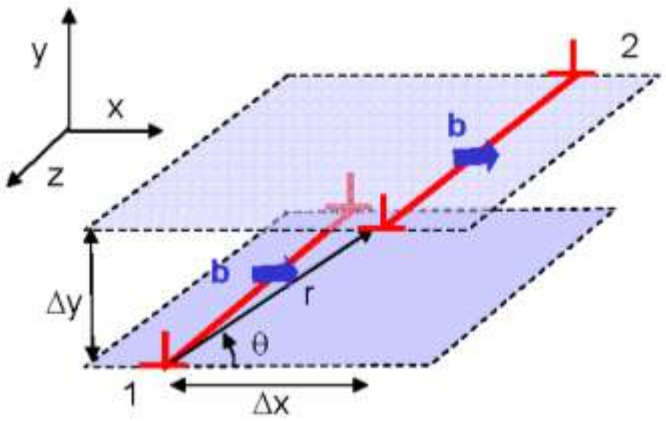
$$\sigma_{xx} = -D\,y\frac{3\Delta x^2 + \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}, \quad \text{with: } D = \frac{Gb}{2\pi(1-\nu)}$$

$$\sigma_{xy} = \sigma_{yx} = D\,\Delta x\frac{\Delta x^2 - \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}$$

So glide force, resolved onto the slip plane, is:

$$F_{glide} = \frac{Gb^2}{2\pi(1-\nu)}\frac{\Delta x(\Delta x^2 - \Delta y^2)}{\left(\Delta x^2 + \Delta y^2\right)^2}$$





$$\sigma_{xx} = -D\,y\,\frac{3\Delta x^2 + \Delta y^2}{\left(\Delta x^2 + \Delta y^2\right)^2}, \quad \text{with:} \quad D = \frac{Gb}{2\pi(1-\nu)}$$

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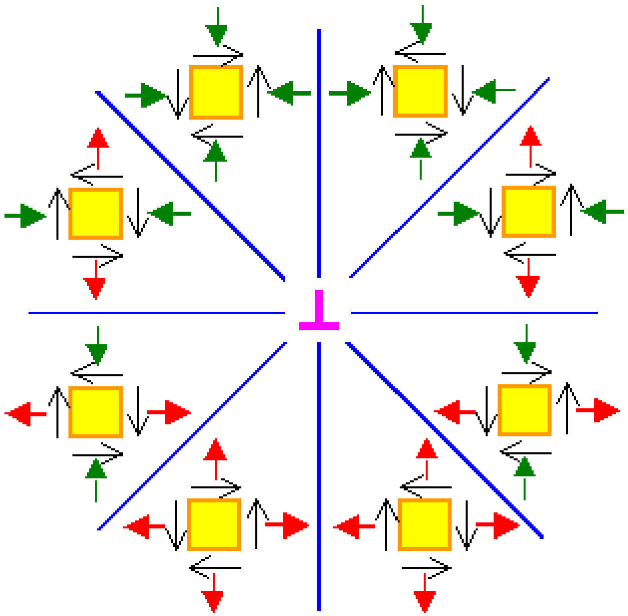
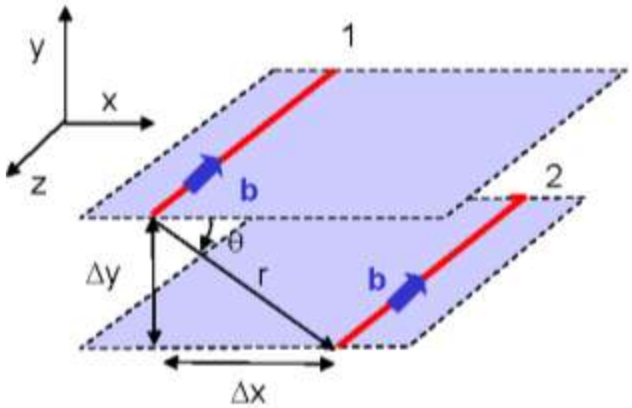


Forces among screw dislocations



Dislocation 2 "feels" the stress field of dislocation 1 (and vice versa).

$$\sigma_{\theta z} = \sigma_{z\theta} = \frac{Gb}{2\pi r}$$

So force on dislocation 2 from dislocation 1 is:

$$F = \frac{Gb^2}{2\pi r}$$

… but this force acts in the radial direction.

Force on dislocation 2 from dislocation 1, resolved onto the glide plane is:

$$F_{res} = \frac{Gb^2}{2\pi r}\cos\theta$$

Alternatively, we can use the stress field expressed in Cartesian co-ordinates:

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \sigma_{xy} = \sigma_{yx} = 0$$

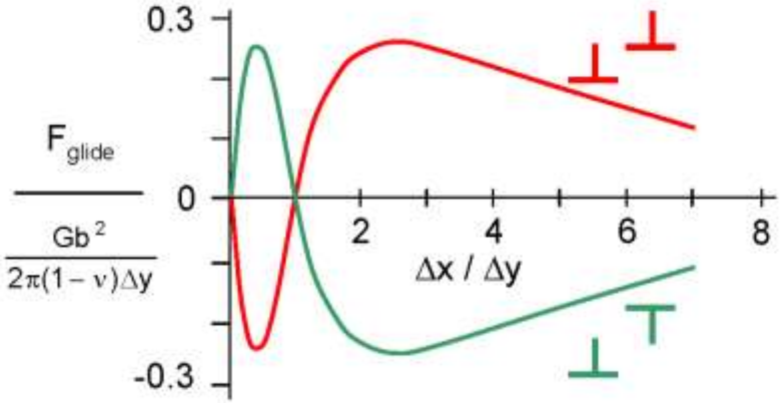
$$\sigma_{xz} = -\frac{Gb}{2\pi}\frac{\Delta y}{\Delta x^2 + \Delta y^2} = -\frac{Gb}{2\pi}\frac{\sin\theta}{r}$$

$$\sigma_{yz} = \frac{Gb}{2\pi}\frac{\Delta x}{\Delta x^2 + \Delta y^2} = \frac{Gb}{2\pi}\frac{\cos\theta}{r}$$

Note that the shear stress acting to shear atoms paralle to **b** above and below the glide plane is σ_{yz}.

$$F_{res} = \sigma_{yz} b = \frac{Gb^2}{2\pi r}\cos\theta = \frac{Gb^2}{2\pi}\frac{\Delta x}{\Delta x^2 + \Delta y^2}$$

Stable configurations for dislocation ensembles



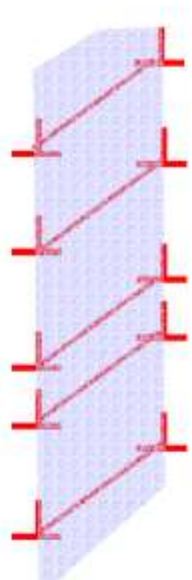
For **like** Burgers vectors:
$\Delta x = \pm\Delta y$: unstable equilibrium
$\Delta x = 0$: stable equilibrium

For **opposite** Burgers vectors:
$\Delta x = \pm\Delta y$: stable equilibrium
$\Delta x = 0$: unstable equilibrium

For **like** Burgers vectors:
Stable array is a planar stack

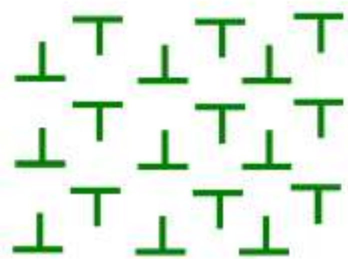
A low angle tilt boundary.

This arrangement has a strong long-range stress field.

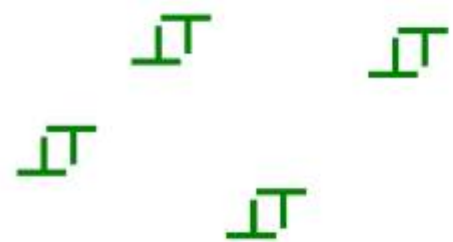


For a set of **"opposite"** Burgers vectors:

There are a large number of possible stable arrangements.



"Taylor lattice"



"Dipole dispersion"

These stable arrangements have minimal *long-range* stress fields.

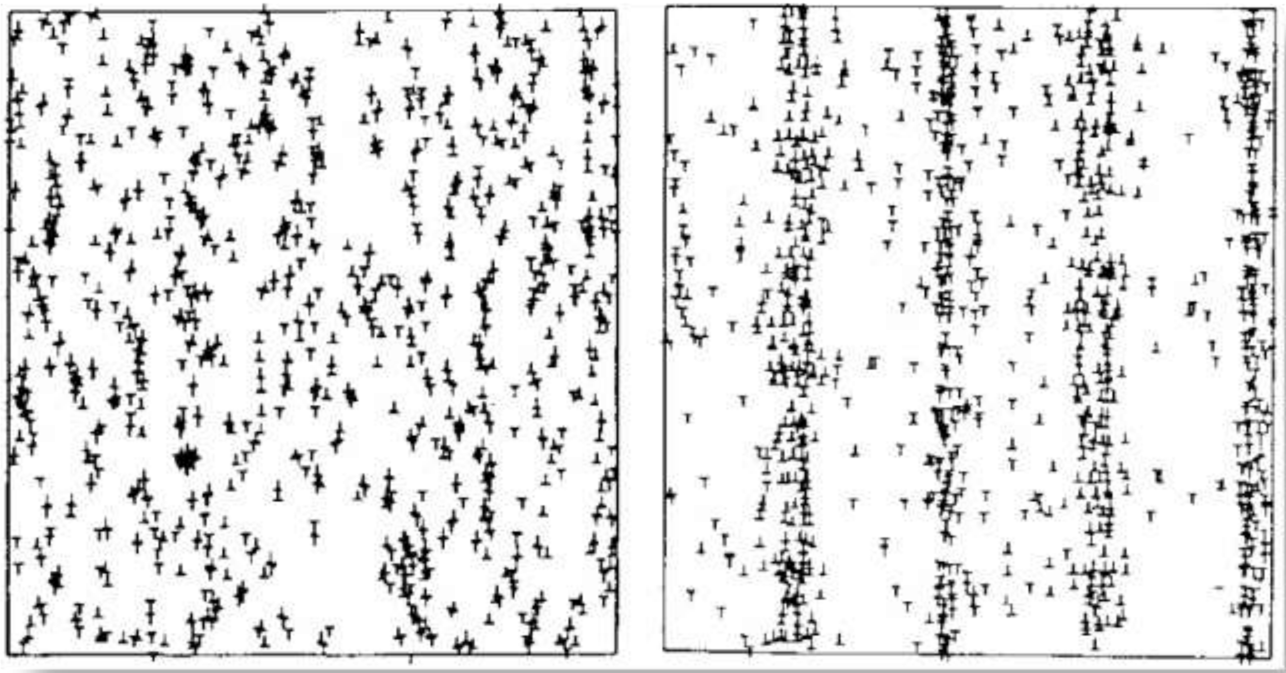
Discrete Dislocation Dynamics

Statistical Dislocation Dynamics

Discrete Dislocation Dynamics

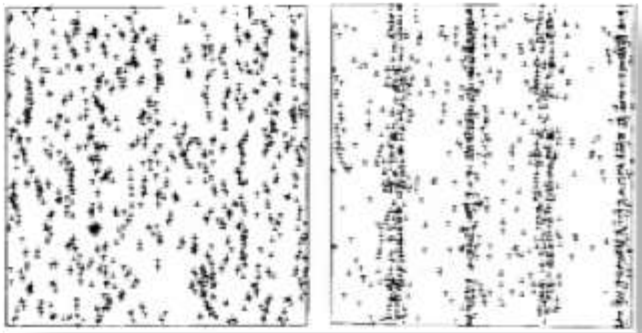
Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line



Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line



Some questions:

Difference between edge and screw dislocations?

How to do multiplication?

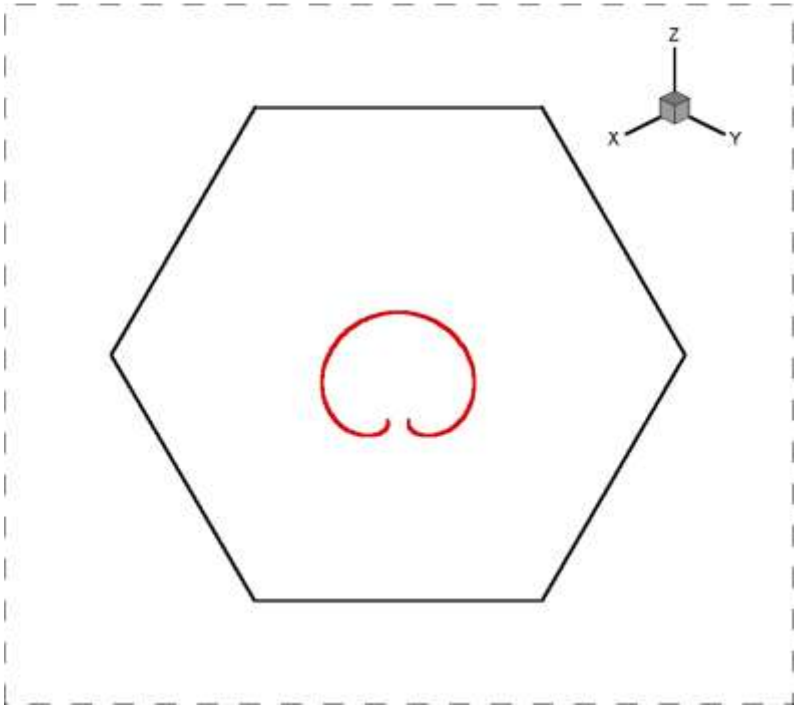
Dislocation bow-out?

Annihilation?

Climbing?

Discrete Dislocation Dynamics in 2D

2D – view into the glide plane



Discrete Dislocation Dynamics in 2D

2D – view into the glide plane

Some questions:

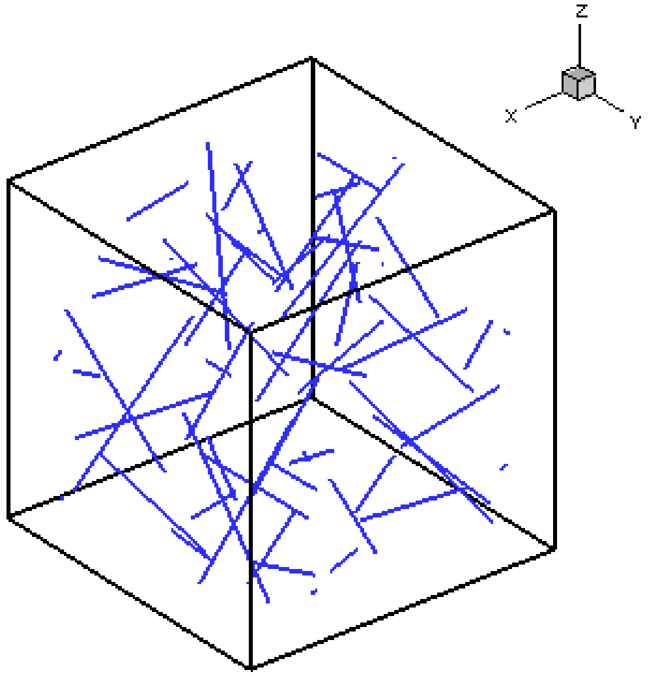
Difference between edge and screw dislocations?

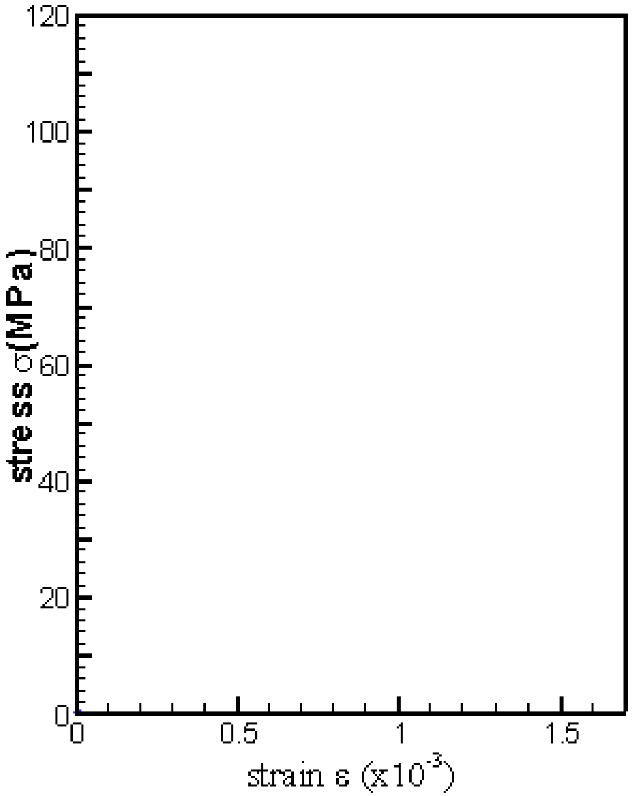
Cross-slip?

Cutting?

Jog-drag?

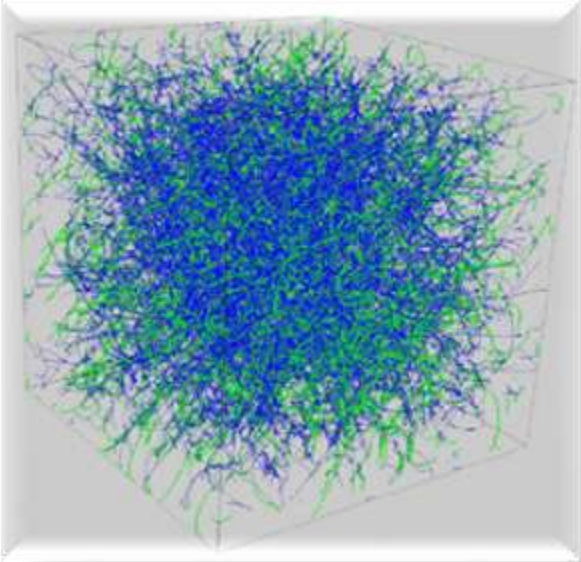
3D: DDD (discrete dislocation dynamics)





Discrete Dislocation Dynamics in 3D

Full 3D segment treatment



Some questions:

Difference between edge and screw dislocations?

Junctions?

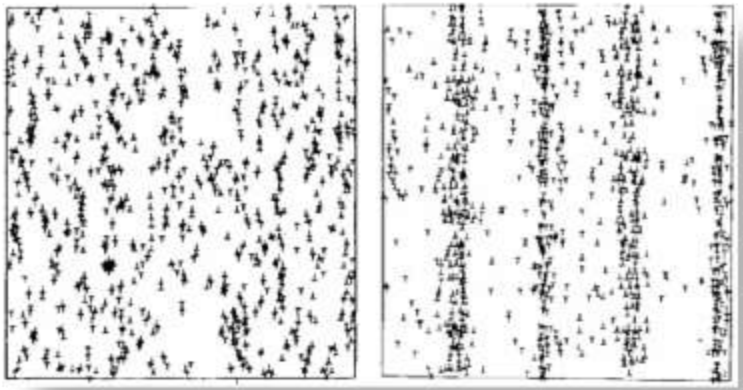
Cutting?

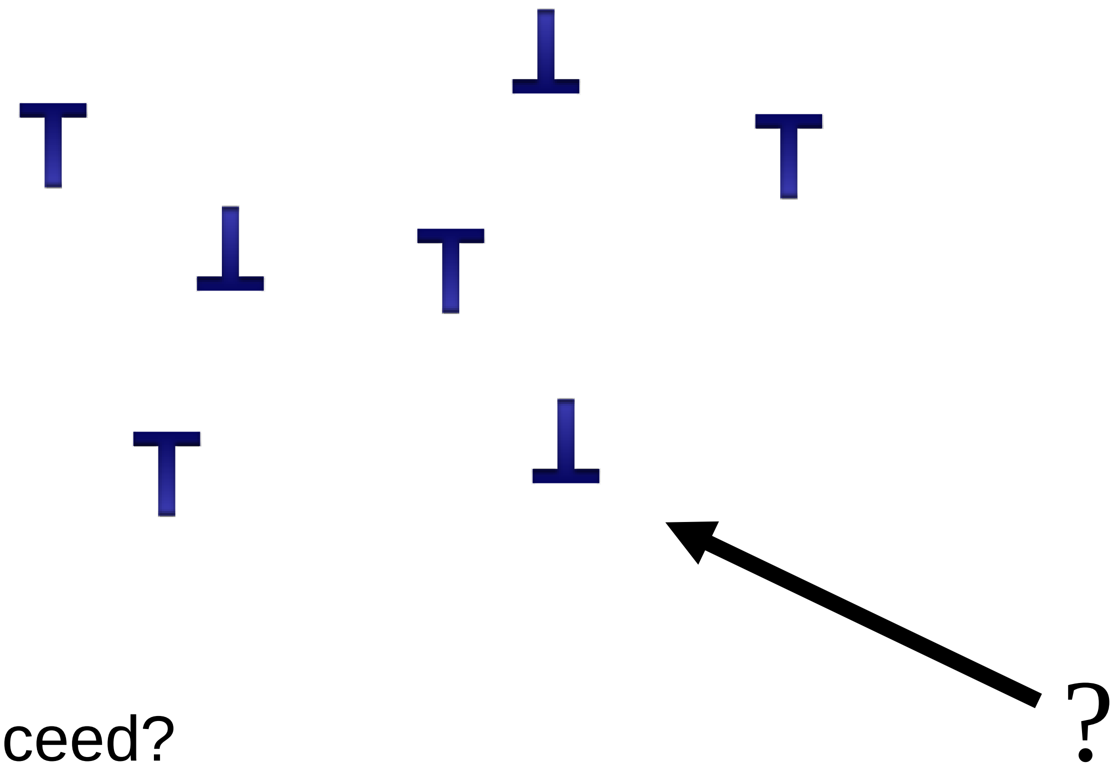
Cores of the dislocations?

Discrete Dislocation Dynamics in 2D

2D – view parallel to dislocation line

Principle procedure





How to proceed?

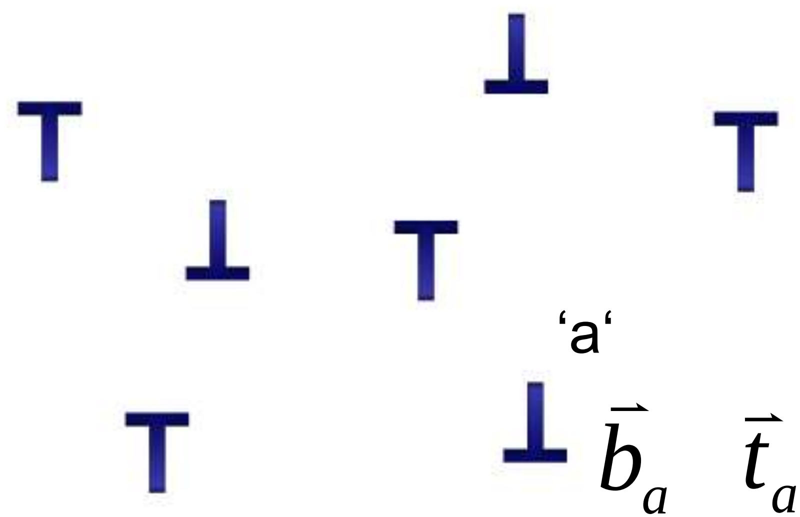
Stress field of (edge) dislocation
Get coordinates
Use Peach Koehler
Move it

Basics of Discrete Dislocation Dynamics in 2D

Force $$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{all others}\to a}\;\vec{b}_a\right)\times\vec{t}_a$$

Force on dislocation ‘a‘

by all others



Force $$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{all others}\to a} \, \vec{b}_a \right) \times \vec{t}_a$$

acceleration   friction coefficient (drag)

Motion $$\vec{F} = m\,\ddot{\vec{x}} + B\dot{\vec{x}} \approx B\dot{\vec{x}}$$

inertia   velocity

Equilibrium of forces

$$\sum \vec{F}_i = 0$$

$$\sum \vec{F}_i = B\dot{\vec{x}} + \vec{F}_a = 0$$

$$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\mathrm{alle} \rightarrow a} \, \vec{b}_a \right) \times \vec{t}_a$$

Equilibrium of forces

$$\boxed{\sum F = 0}$$

$$\boxed{F_{disloc} + F_{self\ force} + F_{extern} + F_{therm} + F_{viscous} + F_{obstacle} + F_{Peierls} + F_{osmotic} + F_{image} + F_{inertia}}$$

F_{disloc} : elastic – other dislocations

$F_{self\ force}$: elastic – self

F_{extern} : external

F_{therm} : Stochastic Langevin

$F_{viscous}$: viscous drag

$F_{obstacle}$: obstacle

$F_{Peierls}$: Peierls

$F_{osmotic}$: chemical forces

F_{image} : surface forces

Example of Discrete Dislocation Dynamics in 2D

$$\sigma_{xz} = \sigma_{zx} = \sigma_{yz} = \sigma_{zy} = 0$$

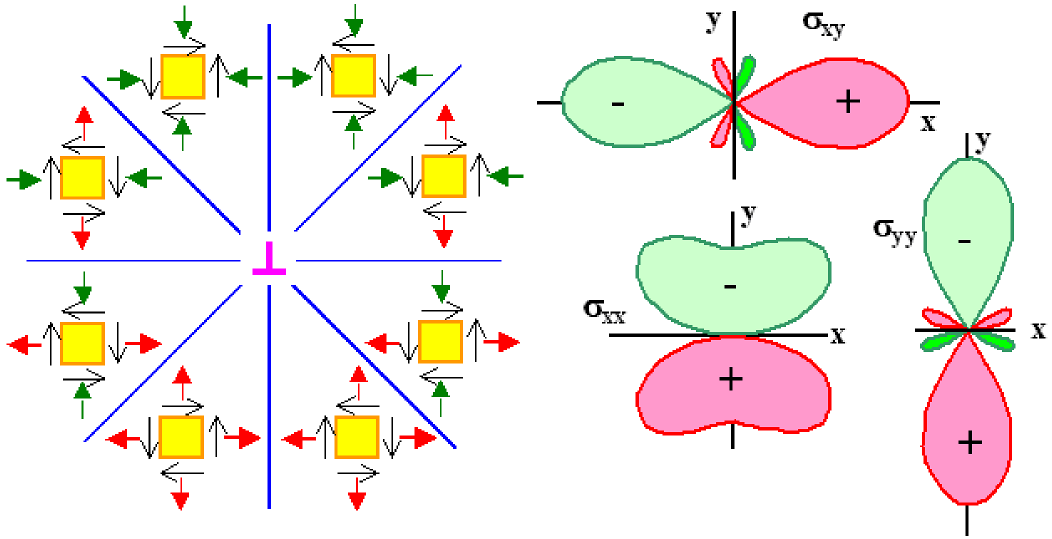
$$\sigma_{xx} = -D\,y\frac{3x^2 + y^2}{\left(x^2 + y^2\right)^2}, \qquad \text{with}: \quad D = \frac{Gb}{2\pi(1-\nu)}$$

$$\sigma_{yy} = D\,y\frac{x^2 - y^2}{\left(x^2 + y^2\right)^2}$$

$$\sigma_{xy} = \sigma_{yx} = D\,x\frac{x^2 - y^2}{\left(x^2 + y^2\right)^2}$$

$$\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$$

1



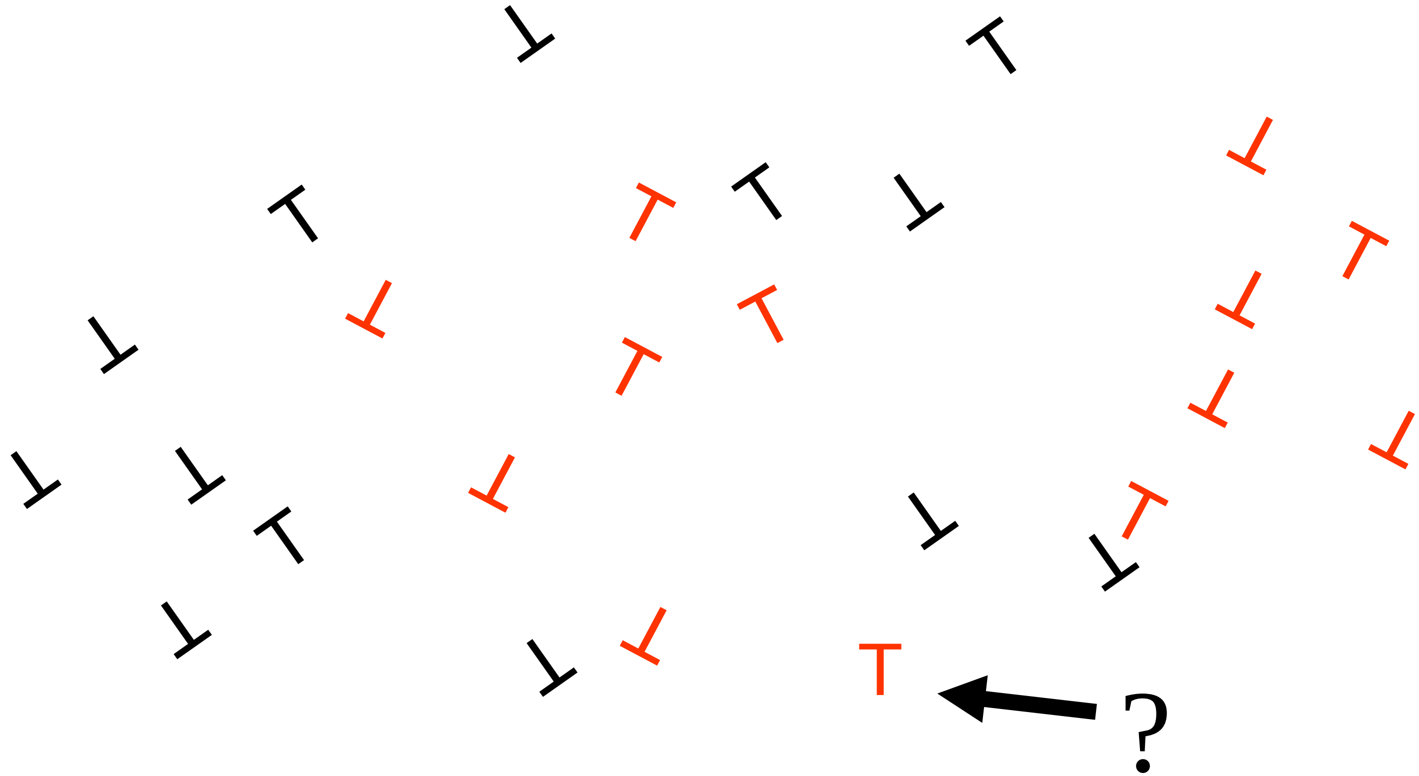
2

$$\vec{F}_a = \left(\underline{\underline{\sigma}}^{\text{all}\rightarrow a}\ \vec{b}_a\right) \times \vec{t}_a$$

3

$$\vec{F}_a + B\dot{\vec{x}} + \vec{F}_{external} = 0$$

Example of Discrete Dislocation Dynamics in 2D



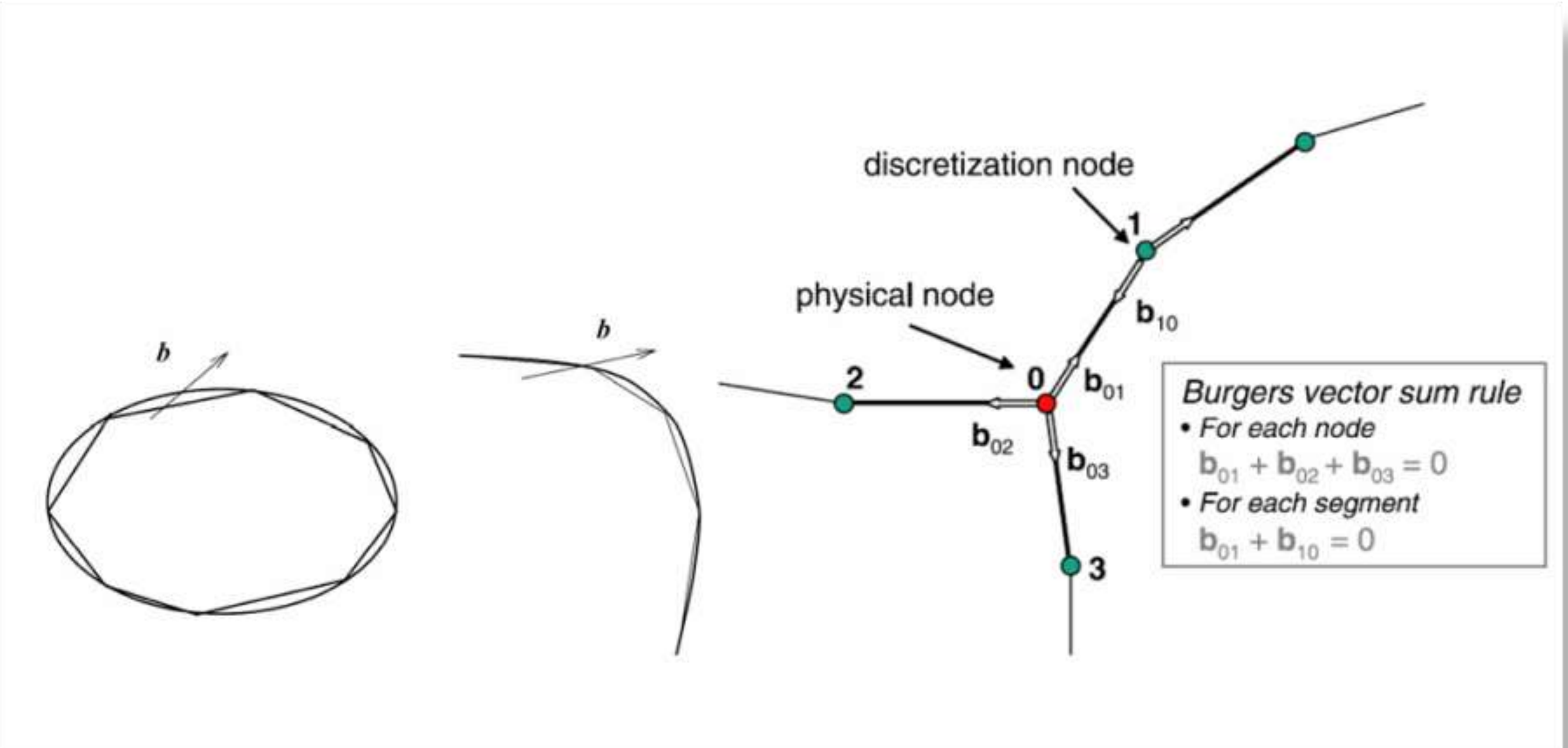
T ← ?

1) Calculate stress field of machine and of all other dislocations at position of T

2) Use Peach-Koehler equation to get force on dislocation

3) Integrate with very small time step (explicit) viscous eq. of motion

3D segments and node construction



Annihilation events

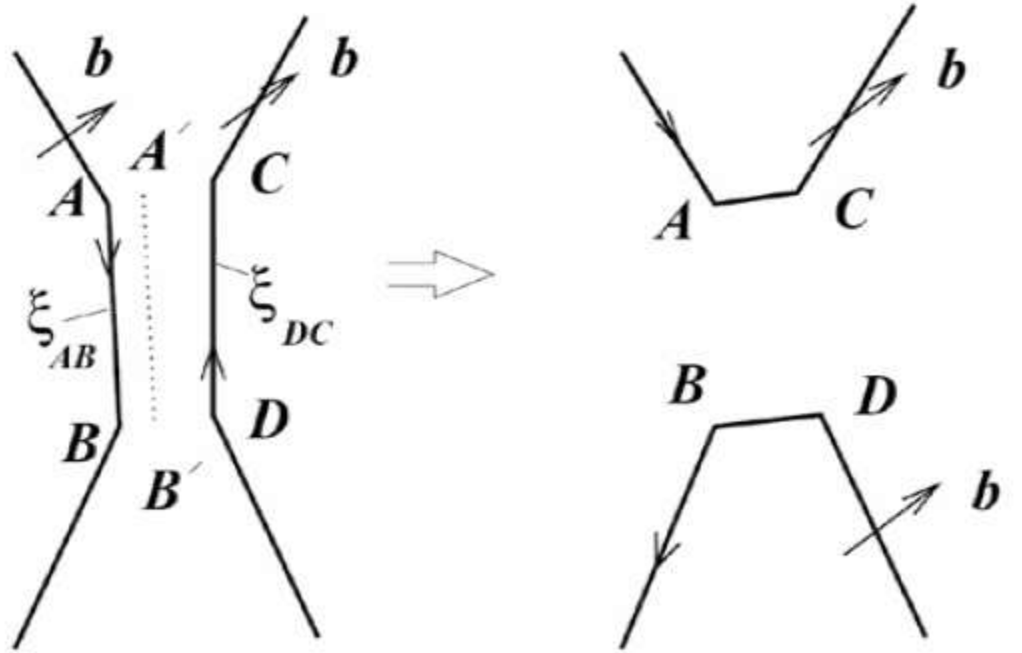


Figure: Annihilation of two attractive dislocations

Jog formation

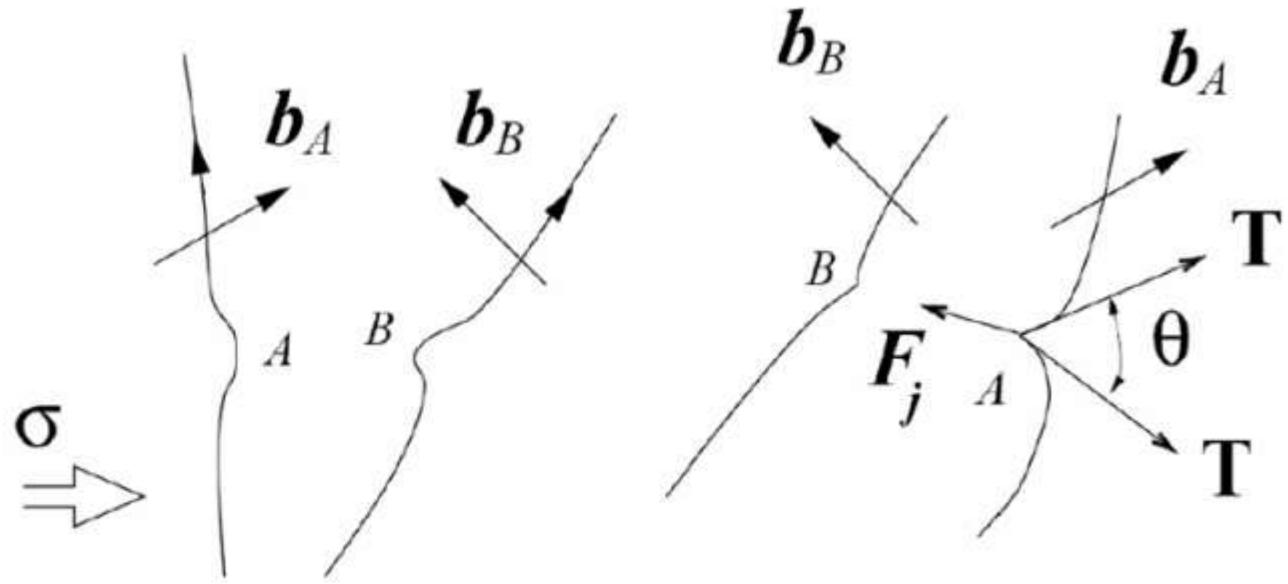
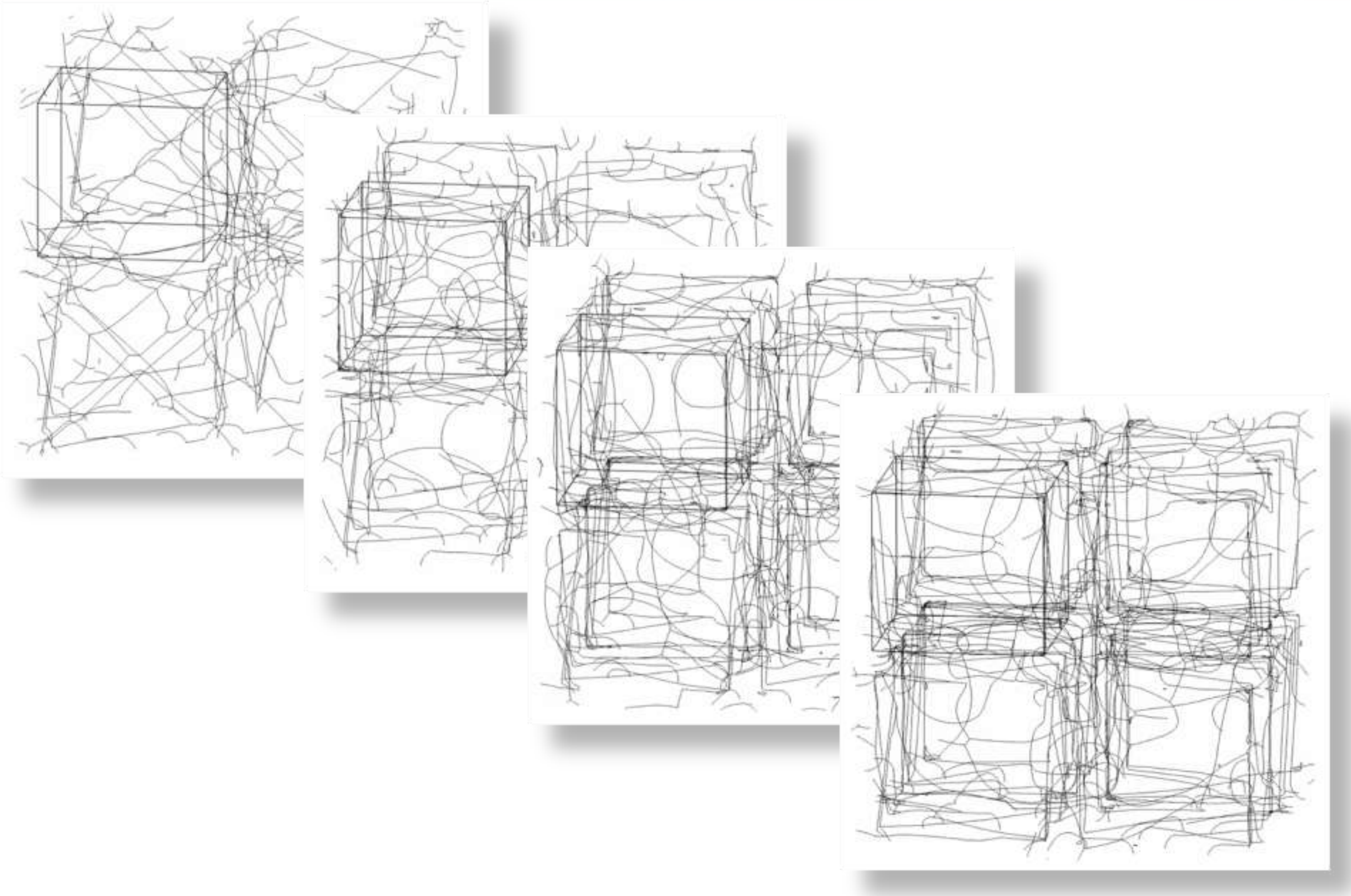
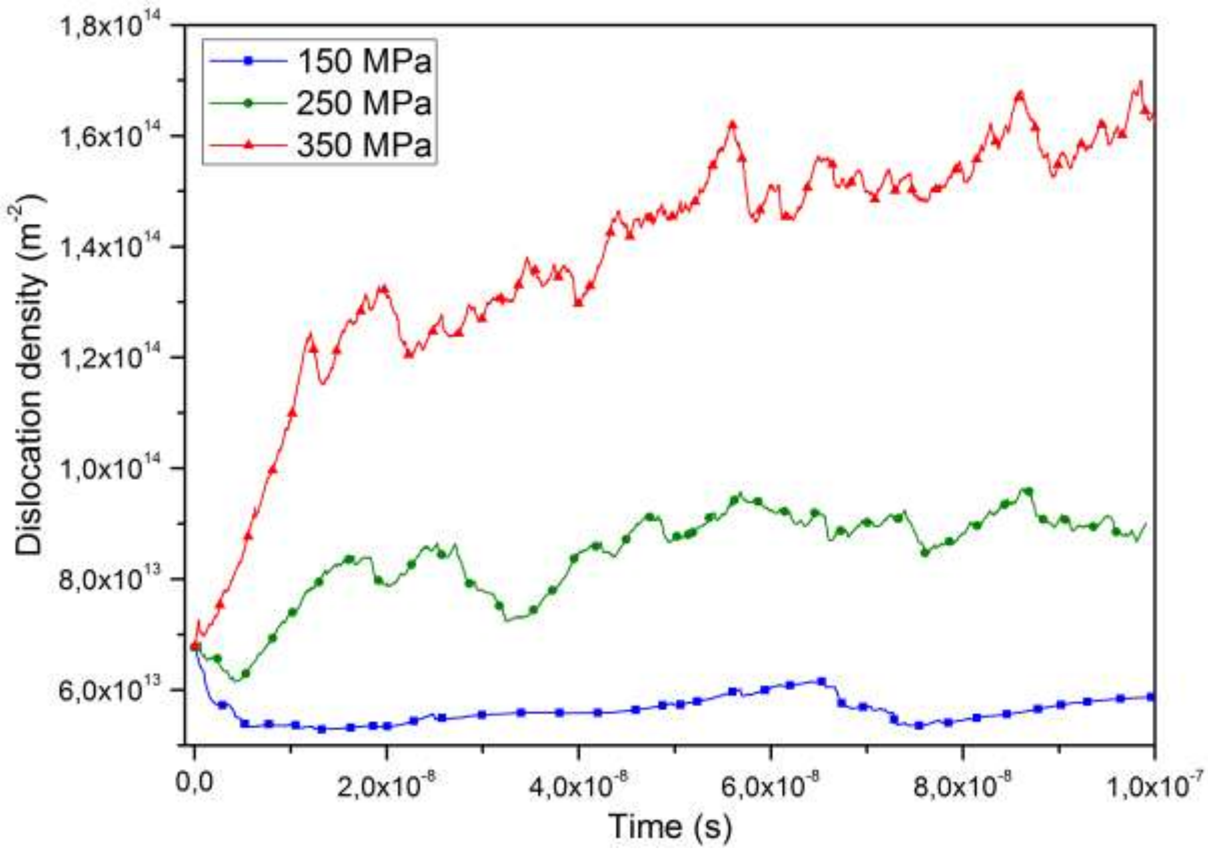


Figure: Jogs are formed when the angle between two attractive dislocations in different planes becomes less than a critical angle θ_c^{jog}

Example of Discrete Dislocation Dynamics in 3D: superalloys

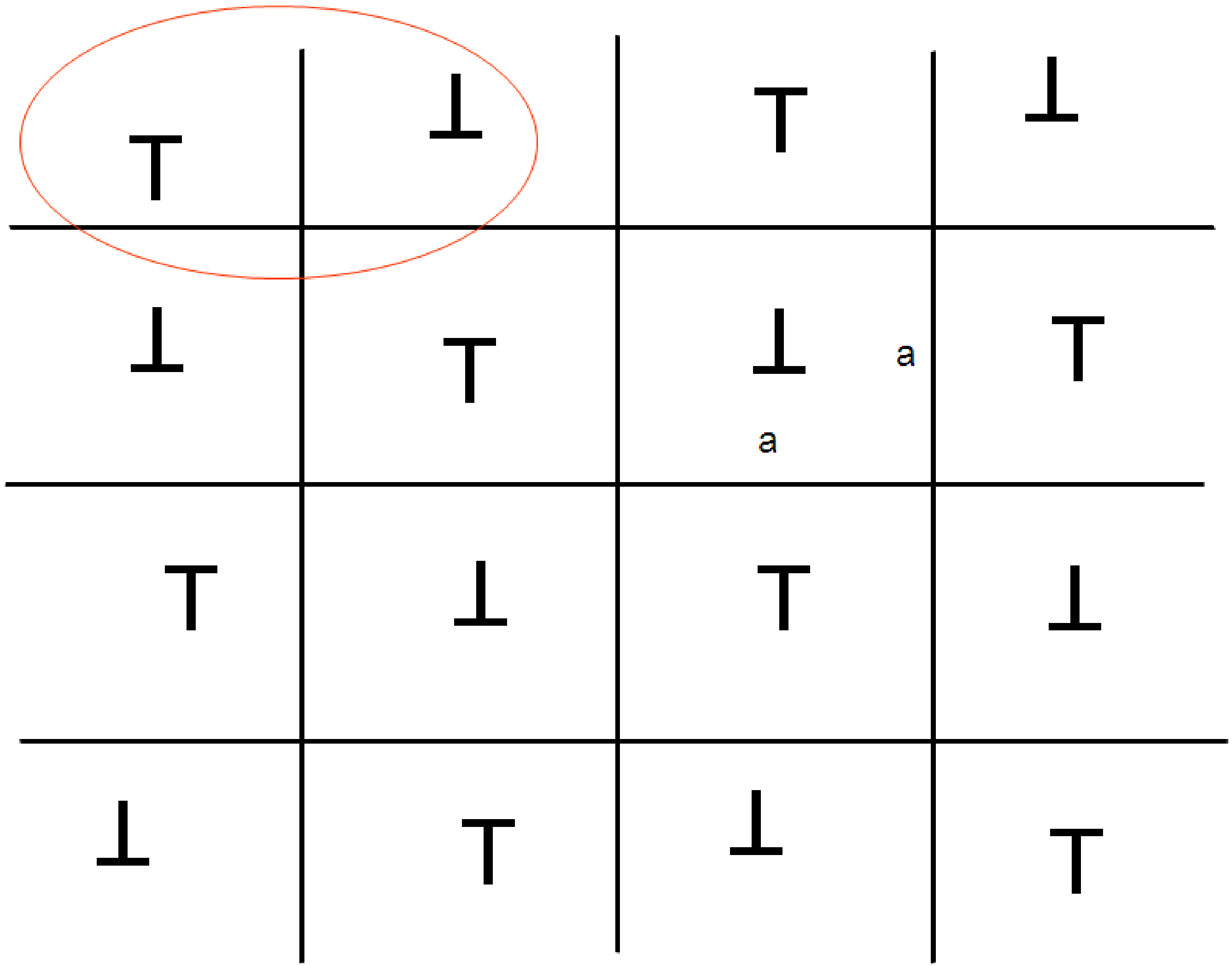


Example of Discrete Dislocation Dynamics in 3D: superalloys



WHY Statistical Dislocation Dynamics ?

- kinetic equation of state
- structure evolution
- coupling to continuum kinematics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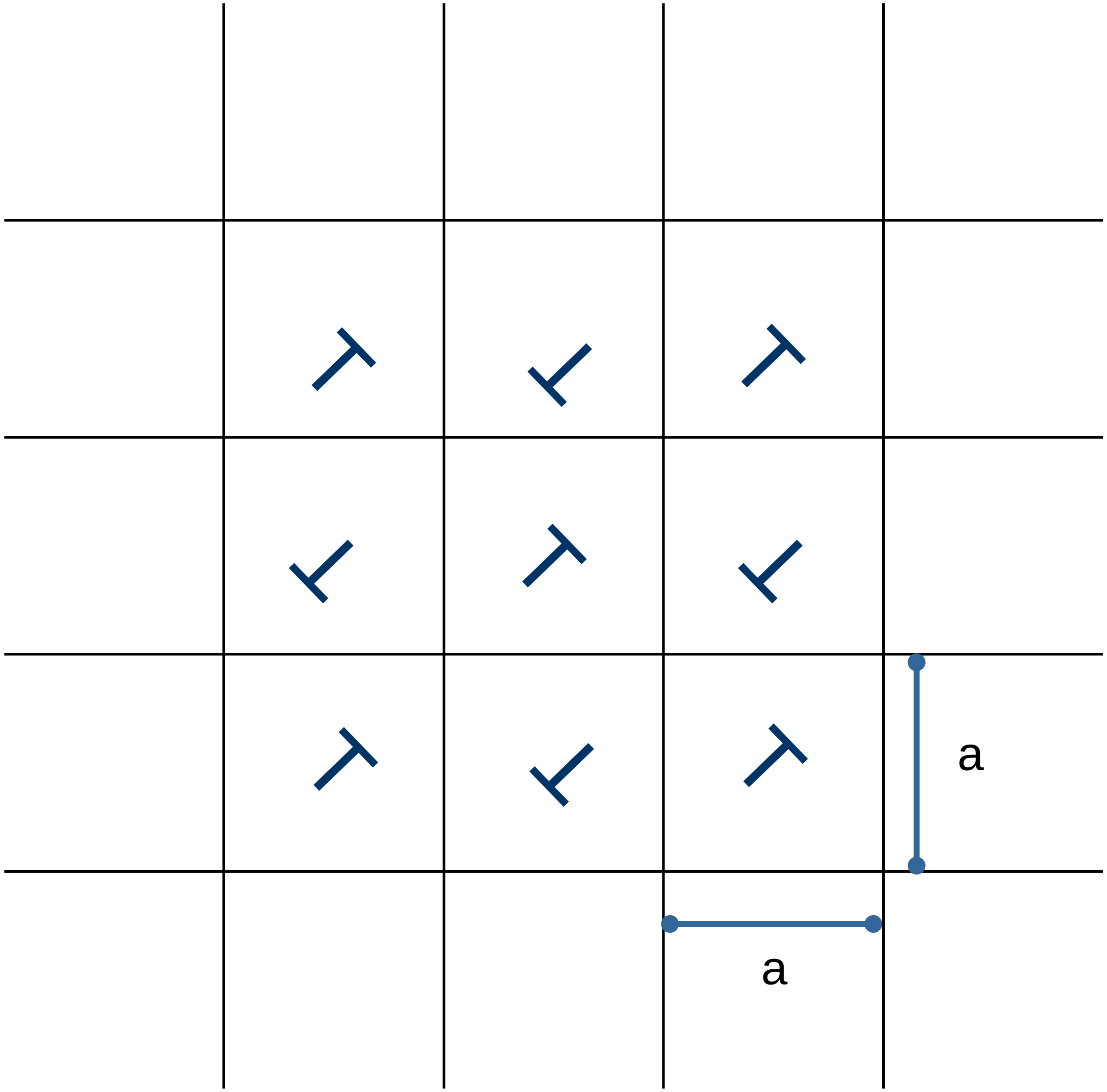
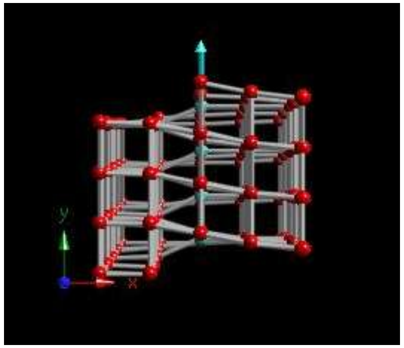


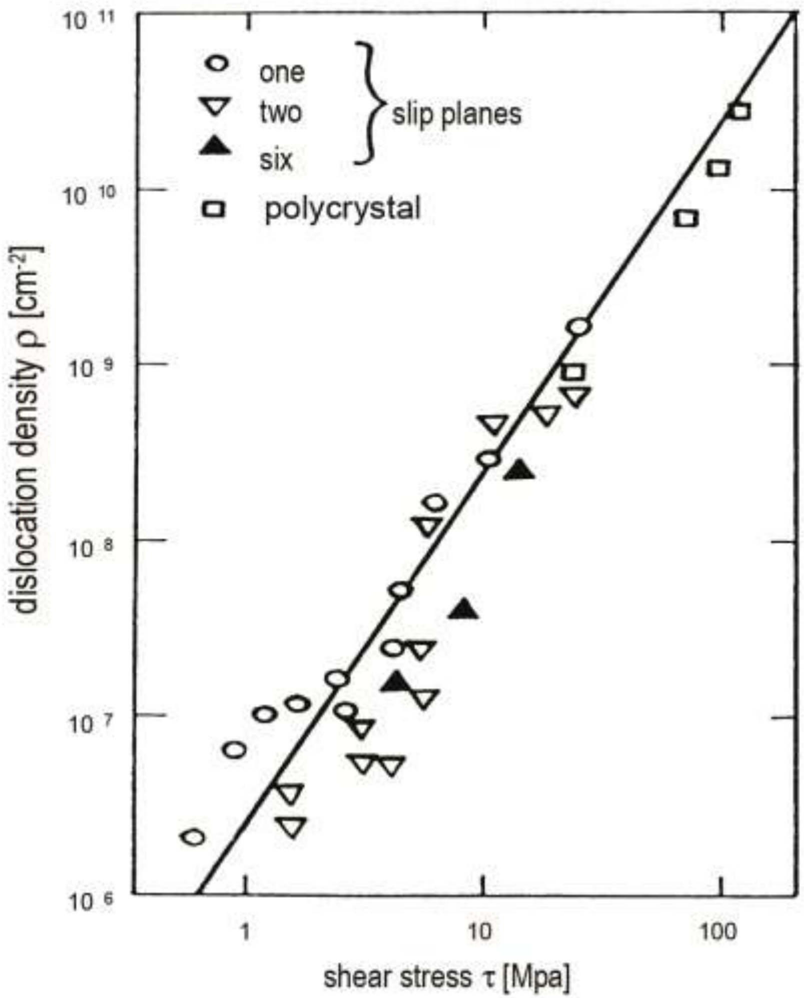


$$\tau = G\gamma = \frac{Gb}{2\pi r}$$

$$\rho = \frac{1}{a^2}$$

$$\tau = \frac{Gb}{2\pi a} = \frac{Gb}{2\pi}\sqrt{\rho}$$

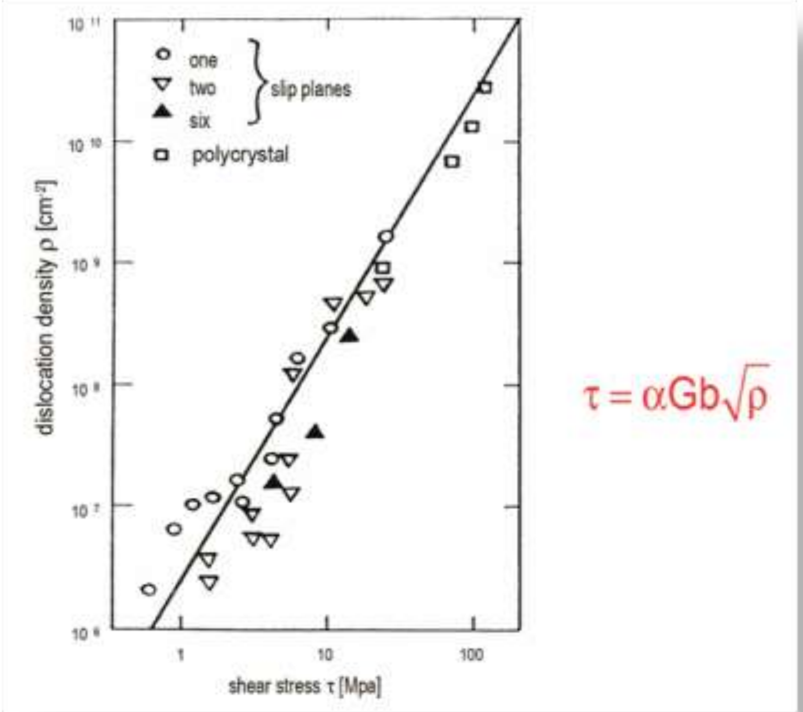
- kinetic equation of state



$$\tau = \alpha G b \sqrt{\rho}$$

kinetics: collective dislocation behaviour

- kinetic equation of state

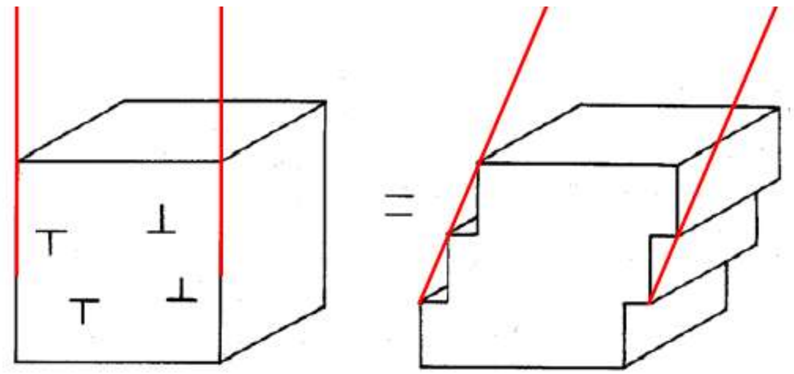


$\tau = \alpha G b \sqrt{\rho}$

- structure evolution

$$\frac{d\rho}{d\gamma} = A\rho^{+} + B\rho^{-}$$

- coupling to imposed shape change



$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$