Class 2007

lecture notes, spring 2007

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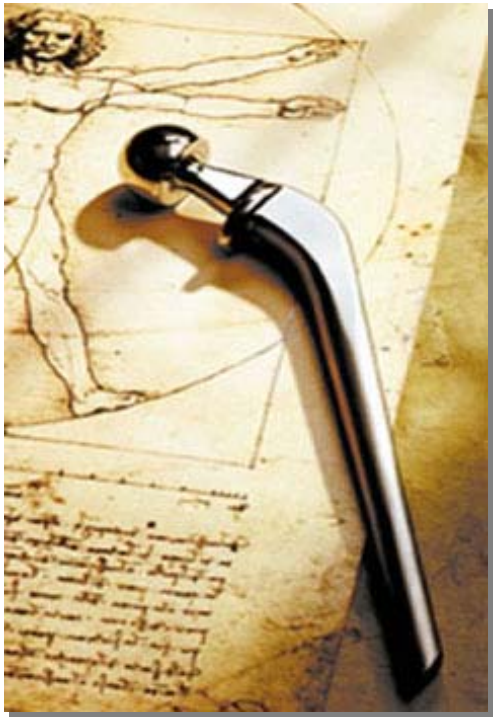
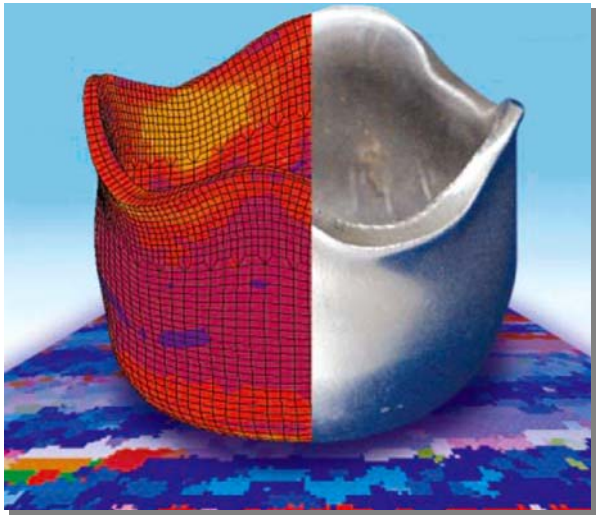
Max-Planck-Institut
Düsseldorf





homework ?

- next Friday:
- class at 9 a.m. at the MPI in Düsseldorf
- see directions on www.mpie.de

Dislocation Dynamics

- **Discrete Dislocation Dynamics**
- **Statistical Dislocation Dynamics**

- **Discrete Dislocation Dynamics**

Basics *(2D, Mode 1)*

Force

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

Motion

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

$$\sum F = 0$$

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

F_{disloc}

elastic - foreign

$F_{self\ force}$

elastic - self

F_{extern}

external

F_{therm}

Stochastic Langevin

$F_{viscous}$

viscous drag

$F_{obstacle}$

obstacle

$F_{Peierls}$

Peierls

$F_{osmotic}$

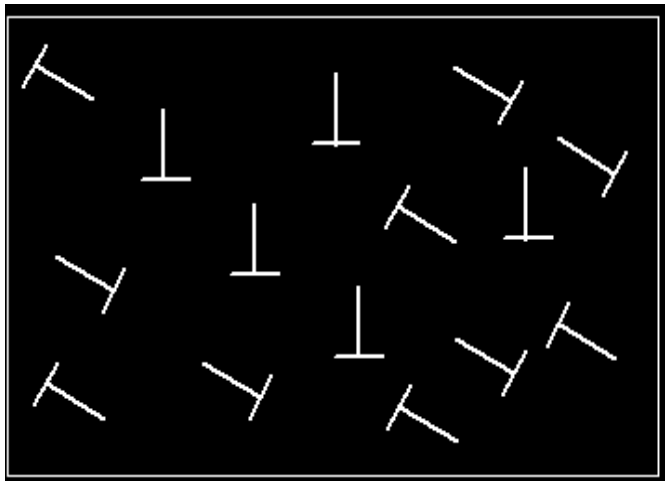
chemical forces

F_{image}

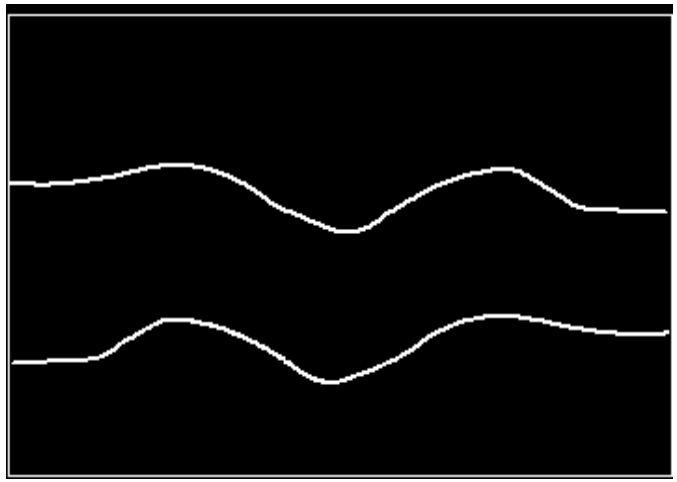
surface forces

Discrete Dislocation Dynamics

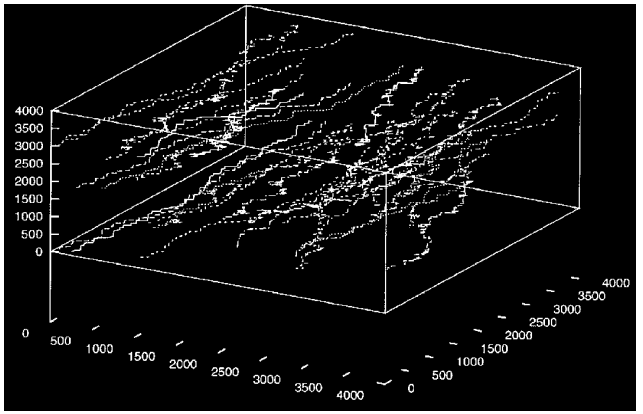
2D - Mode 1



2D - Mode 2



3D



Mode 2 - Example: edge dislocation

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

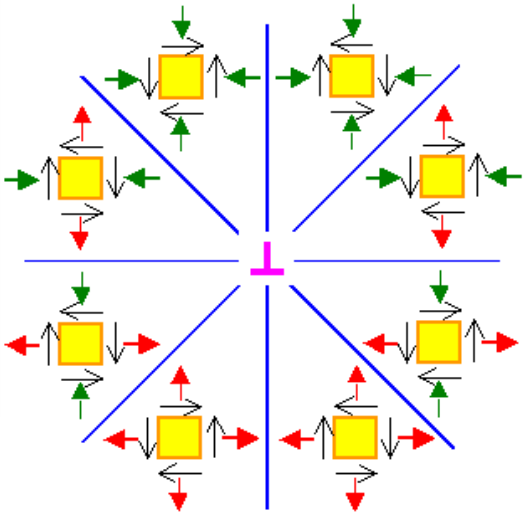
$$\sigma_{xx} = -D\,y\,\frac{3x^2 + y^2}{\left(x^2 + y^2\right)^2}, \qquad \text{with:} \quad D = \frac{Gb}{2\pi(1-\nu)}$$

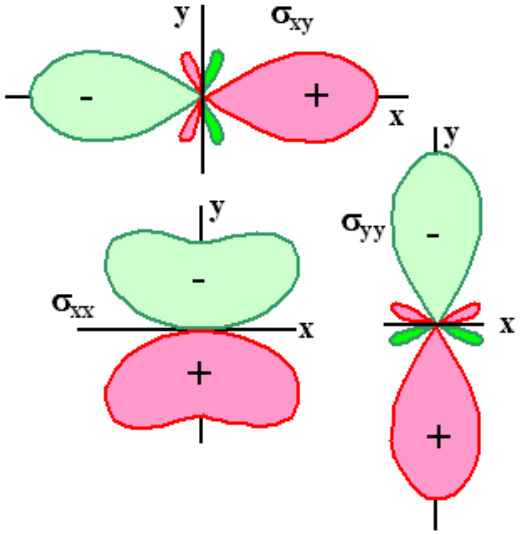
$$\sigma_{yy} = D\,y\,\frac{x^2 - y^2}{\left(x^2 + y^2\right)^2}$$

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

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

1





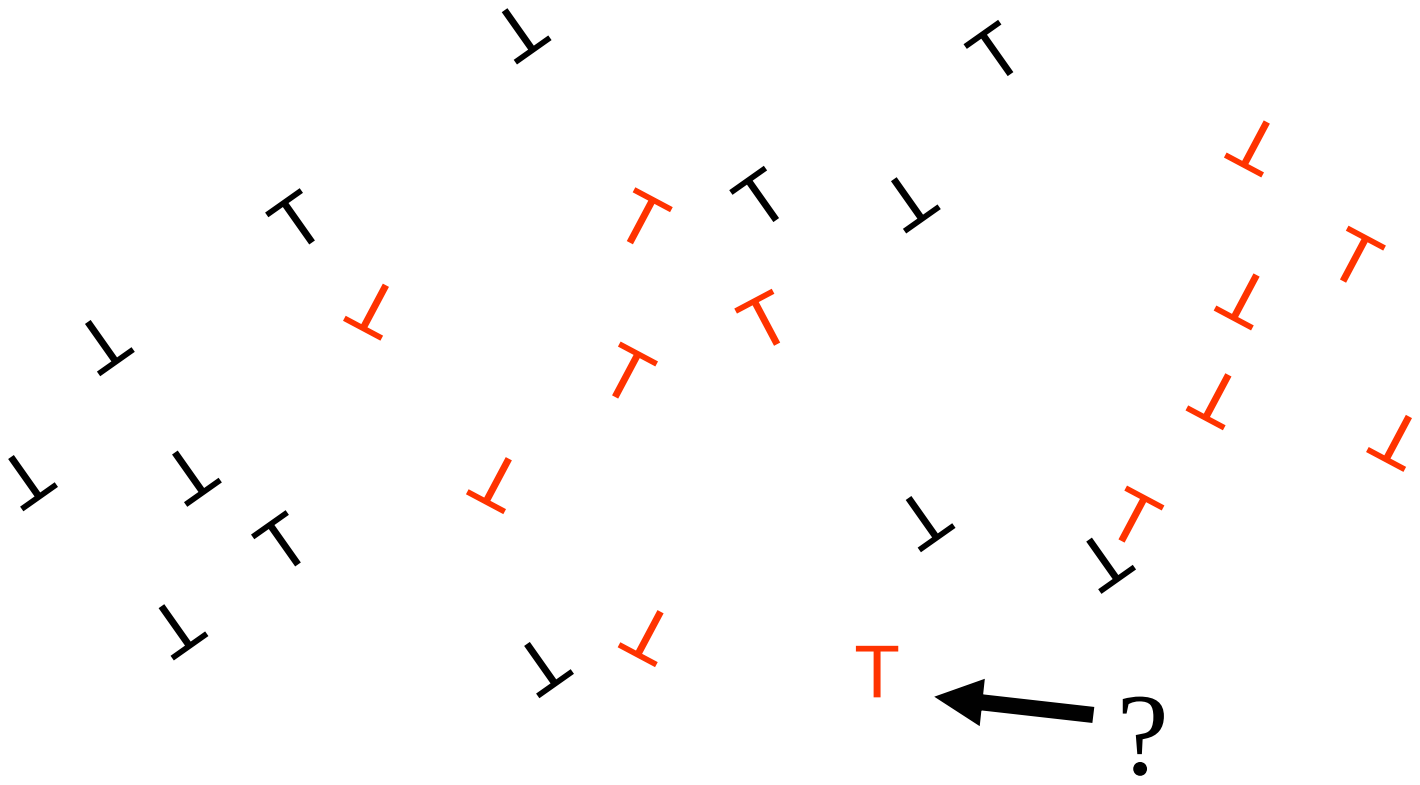
2

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

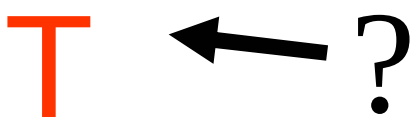
3

$$\vec{F} = B\dot{\vec{x}}$$

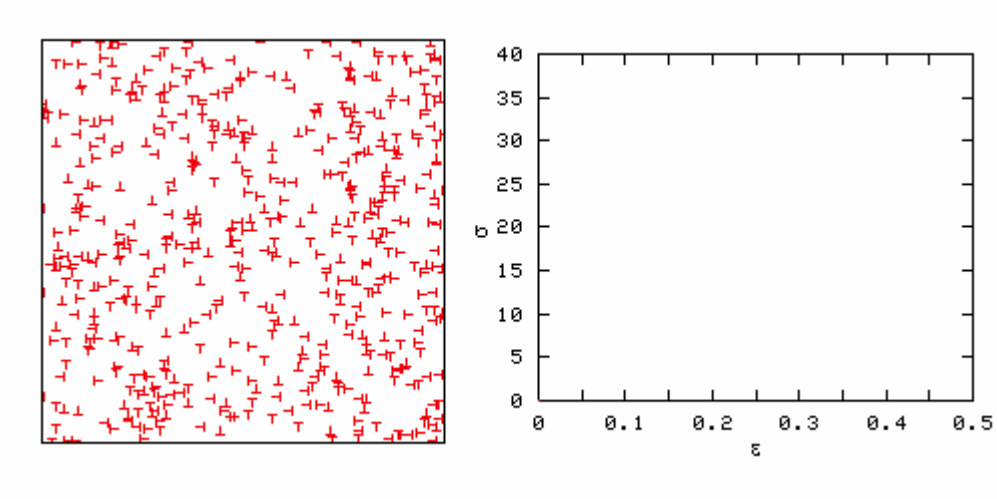
Mode 2 - Example: edge dislocation



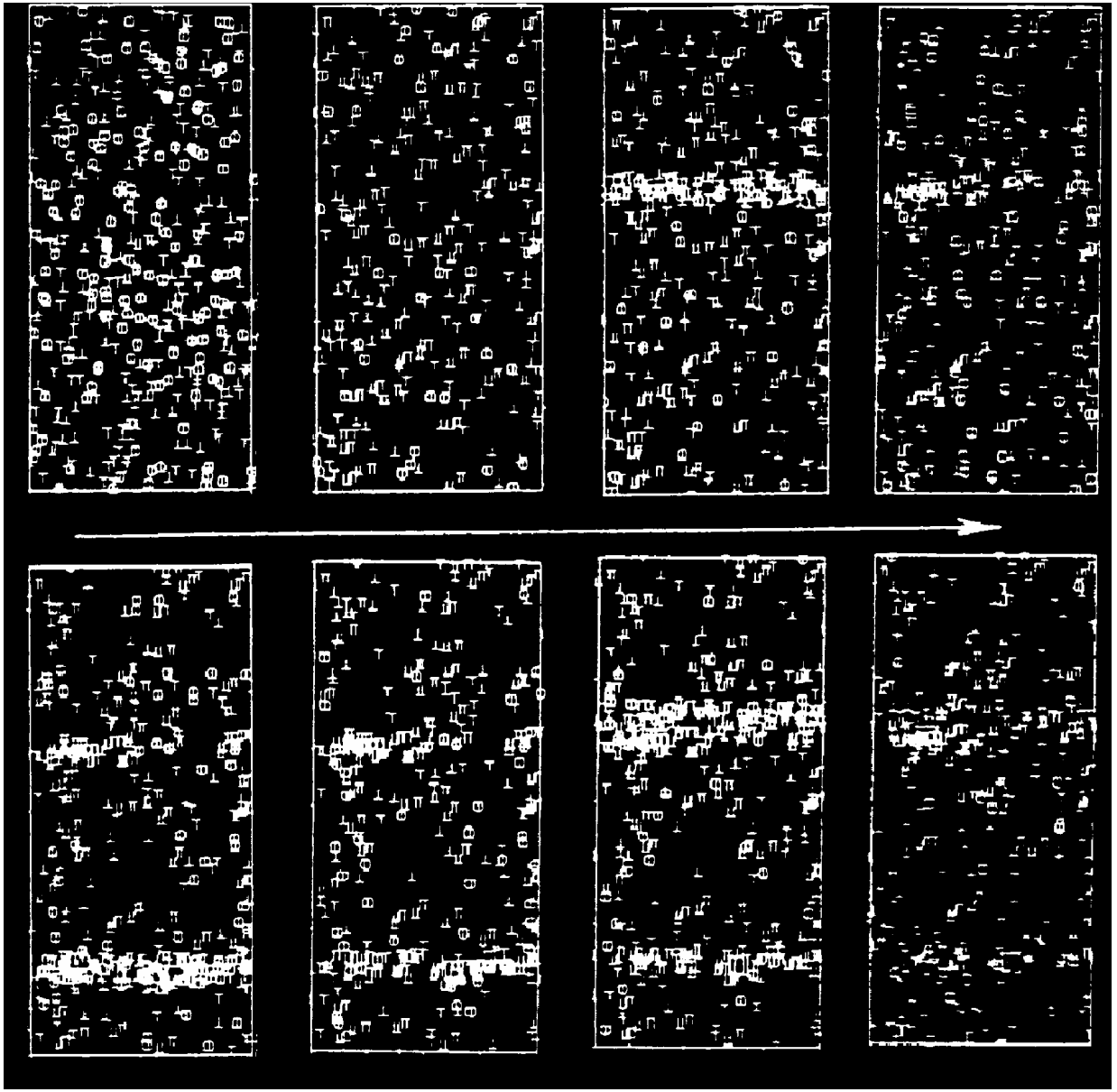
Mode 2 - Example: edge dislocation

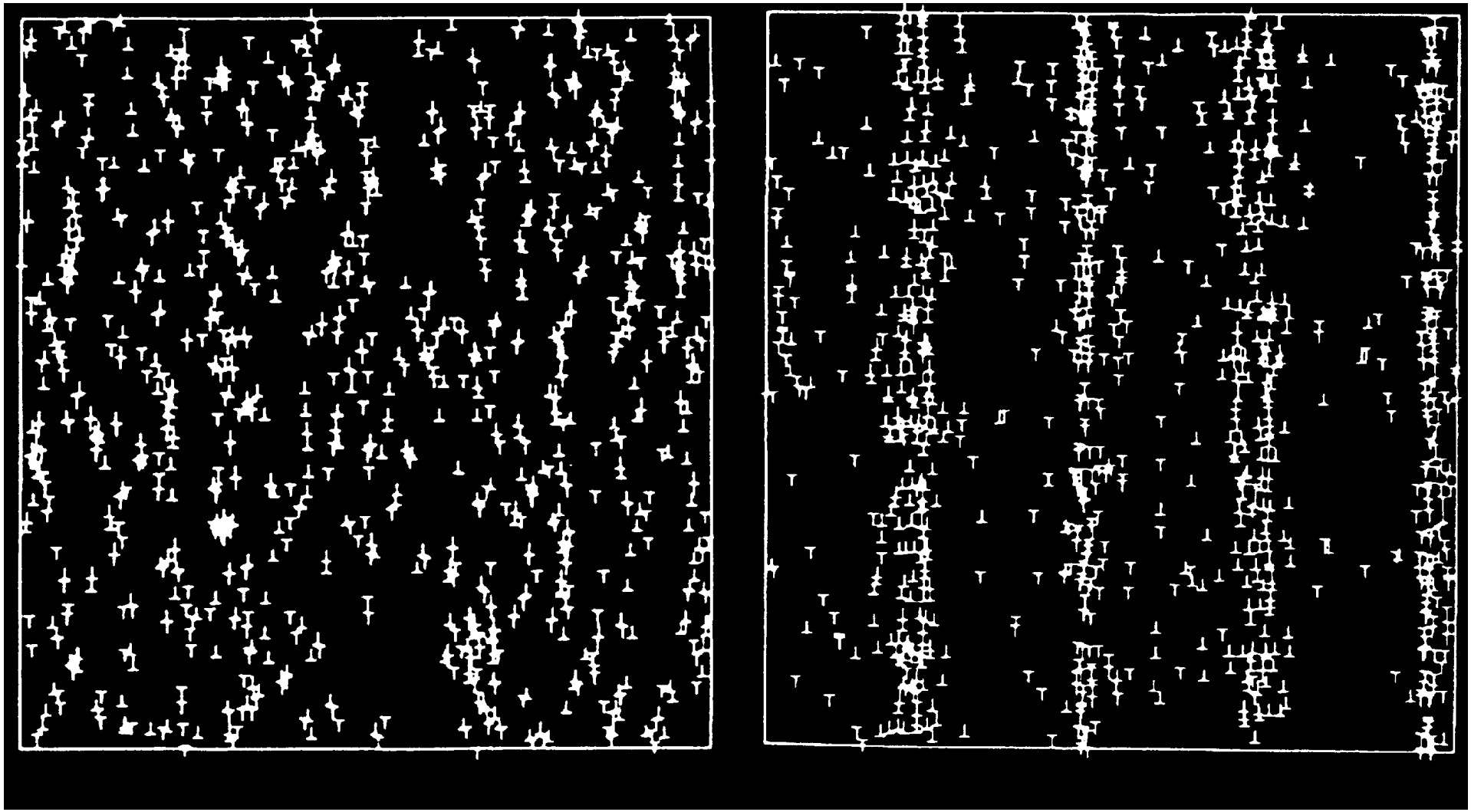


1) calculate stress field of machine and of all other dislocations at position of T
2) Use Peach-Koehler equation to get force on dislocation
3) integrate with very small time step (explicit) viscous eq. of motion

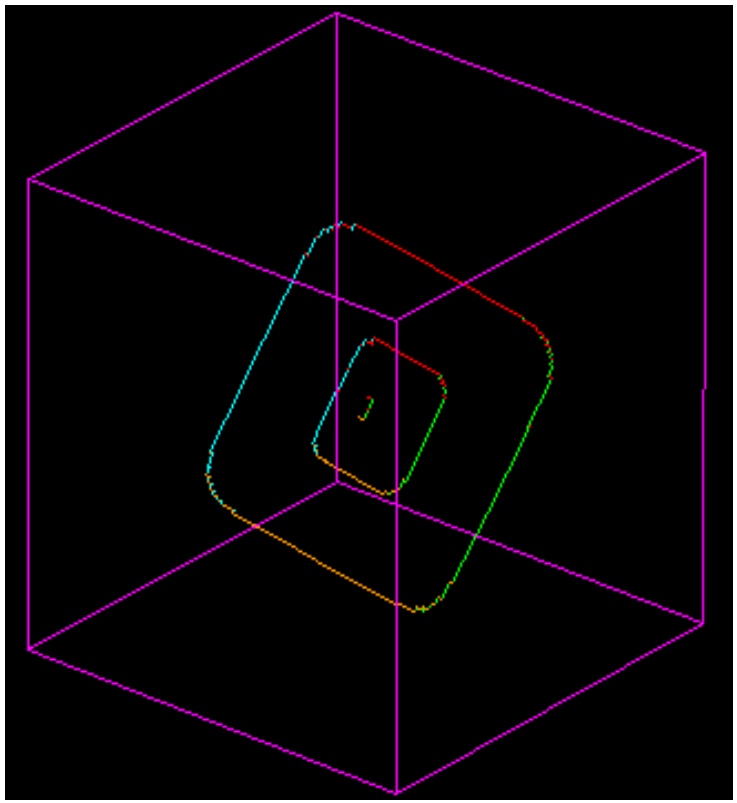

40
35
30
25
20
15
10
5
0
σ
0
0.1
0.2
0.3
0.4
0.5
ε

2D - Mode 1

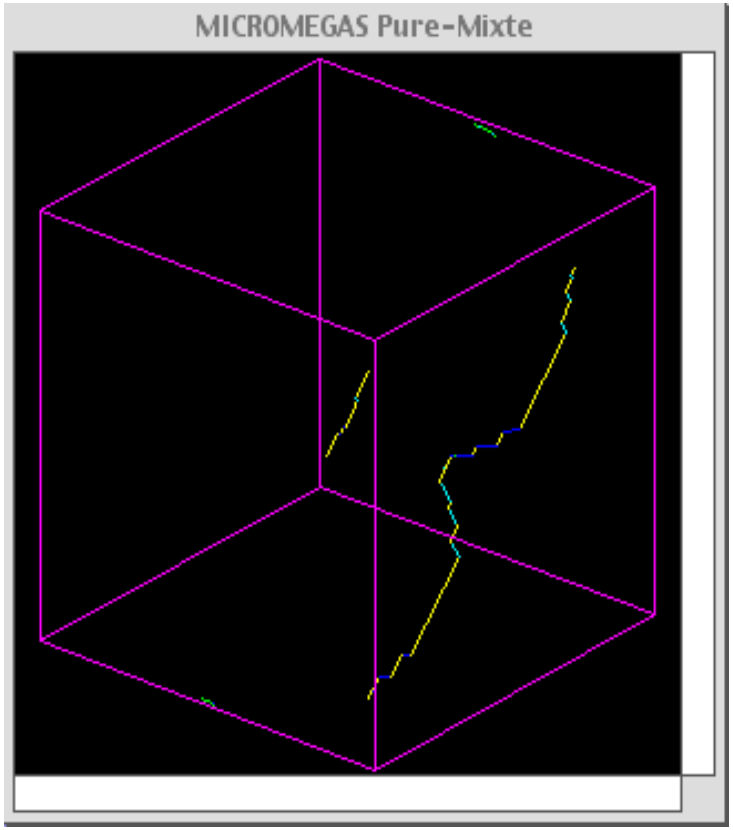




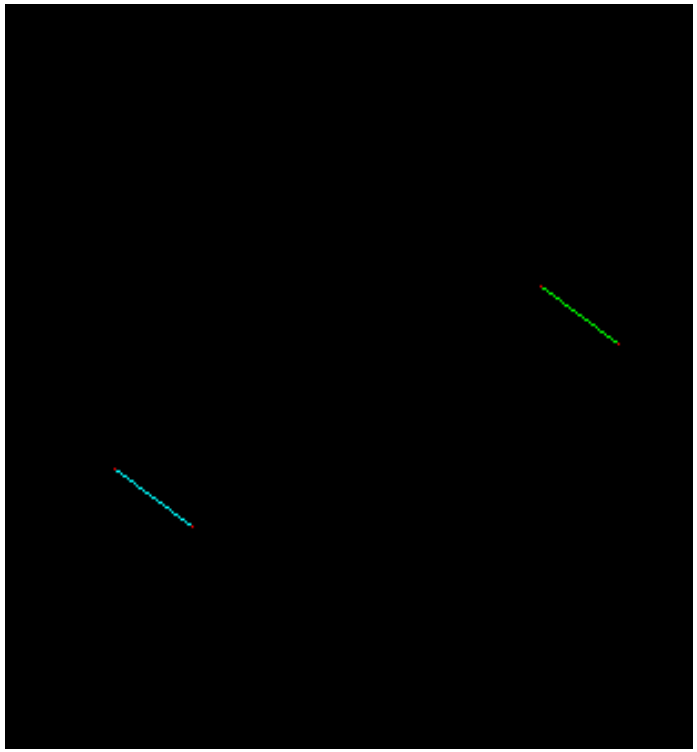
dislocations



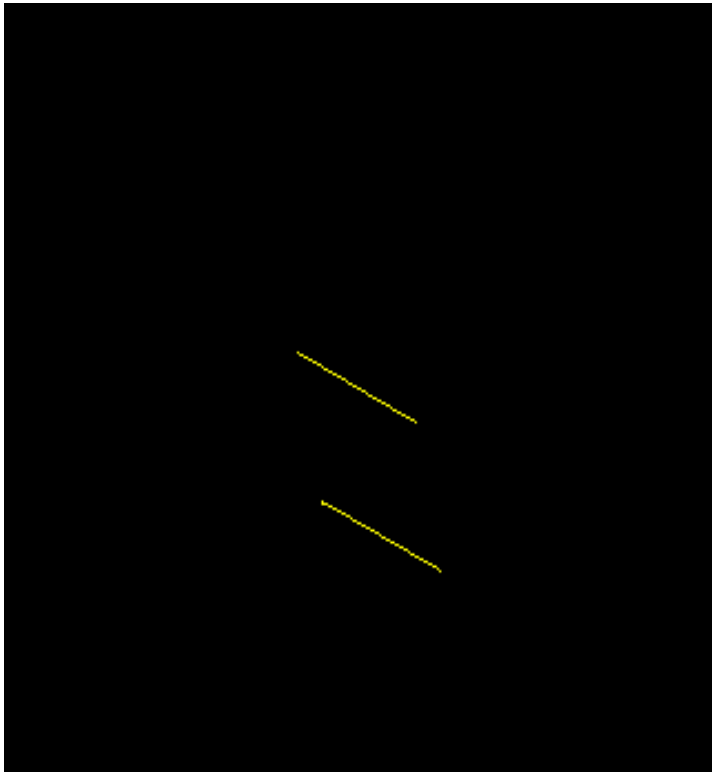
dislocations



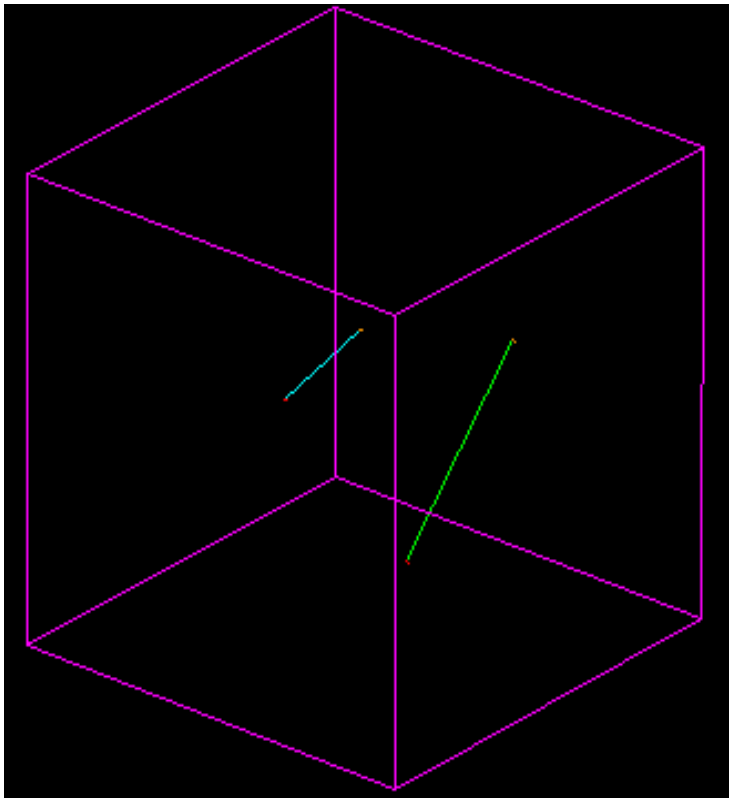
dislocations



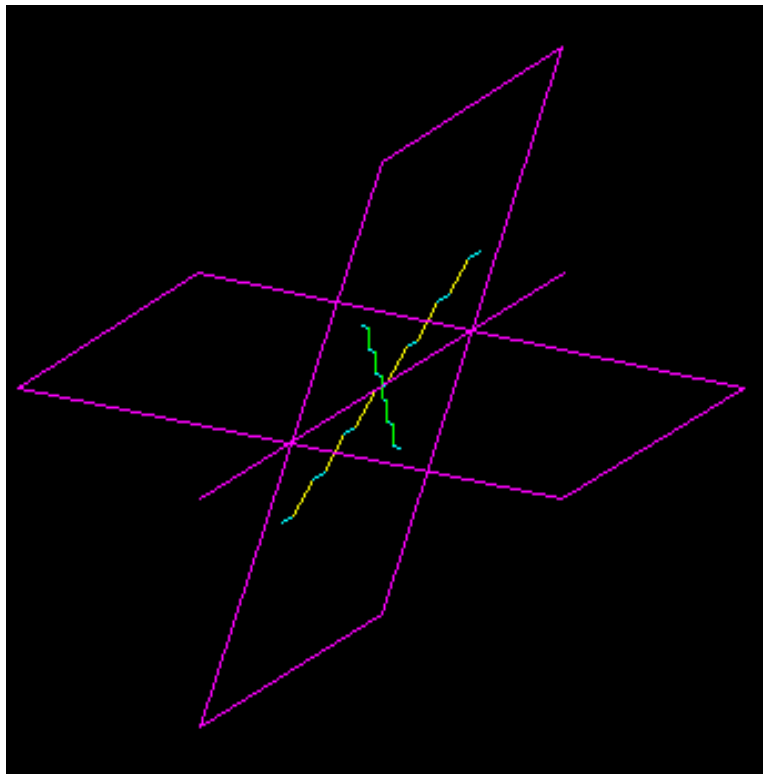
dislocations



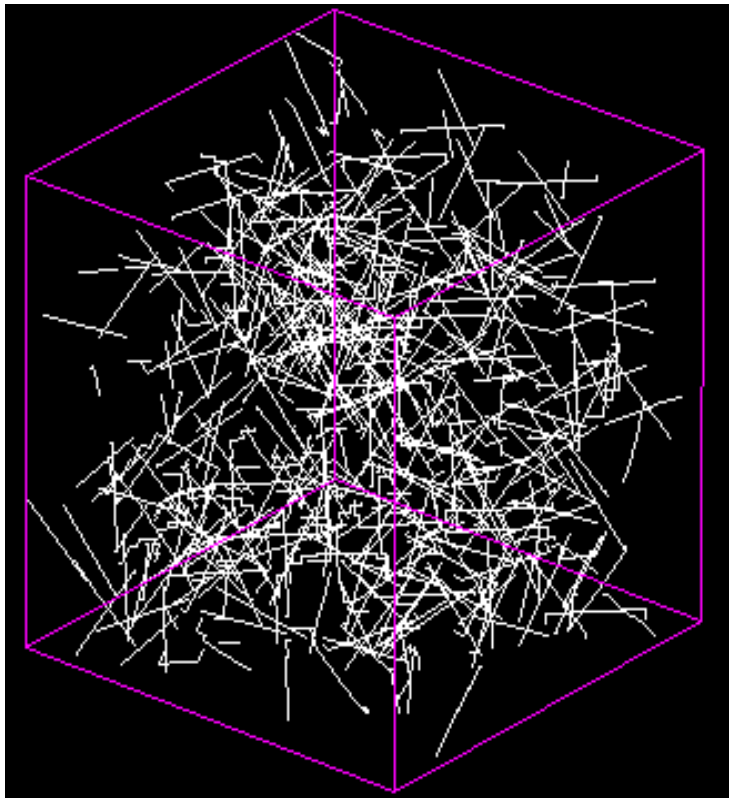
dislocations



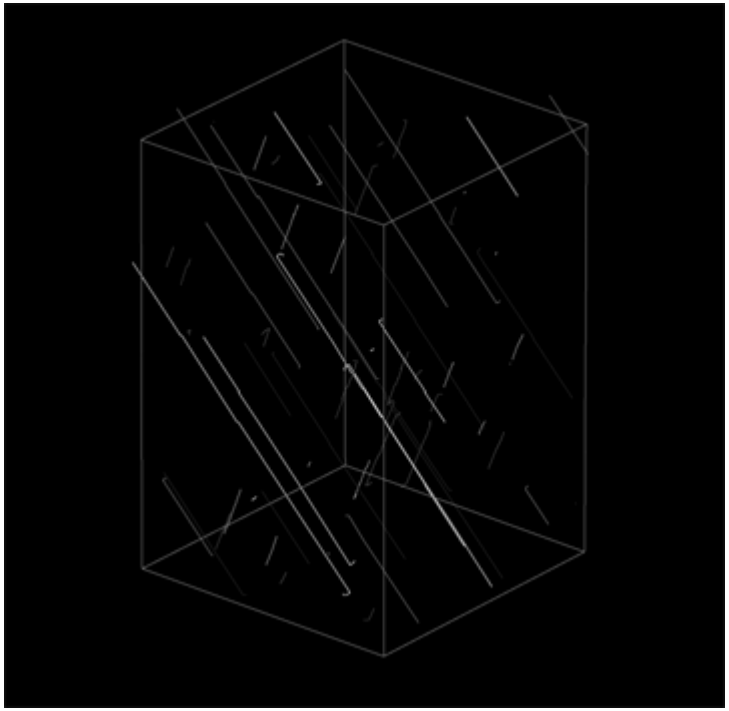
dislocations

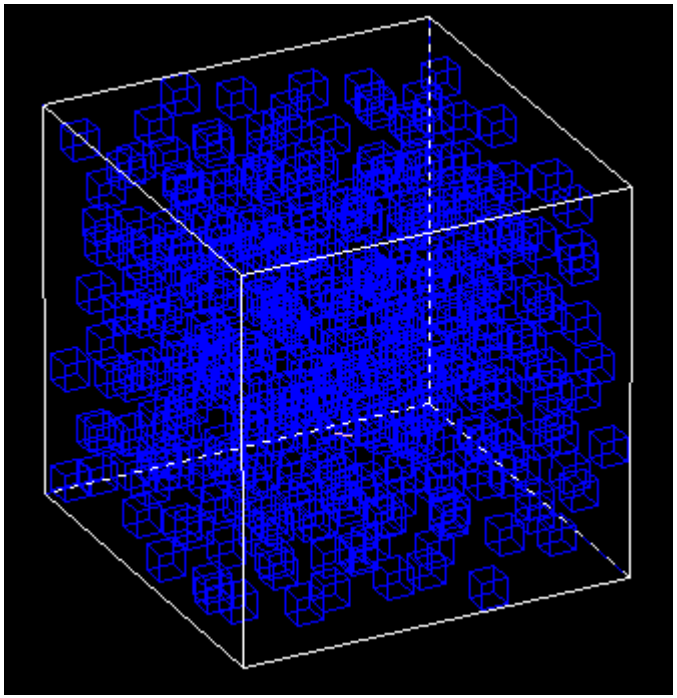


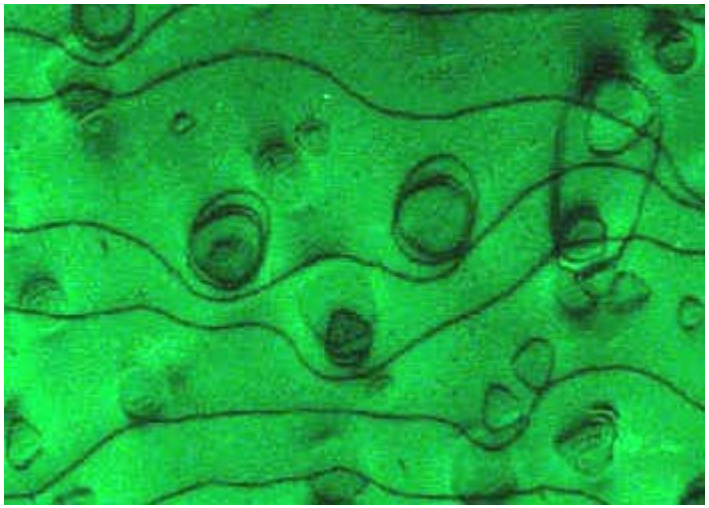
dislocations

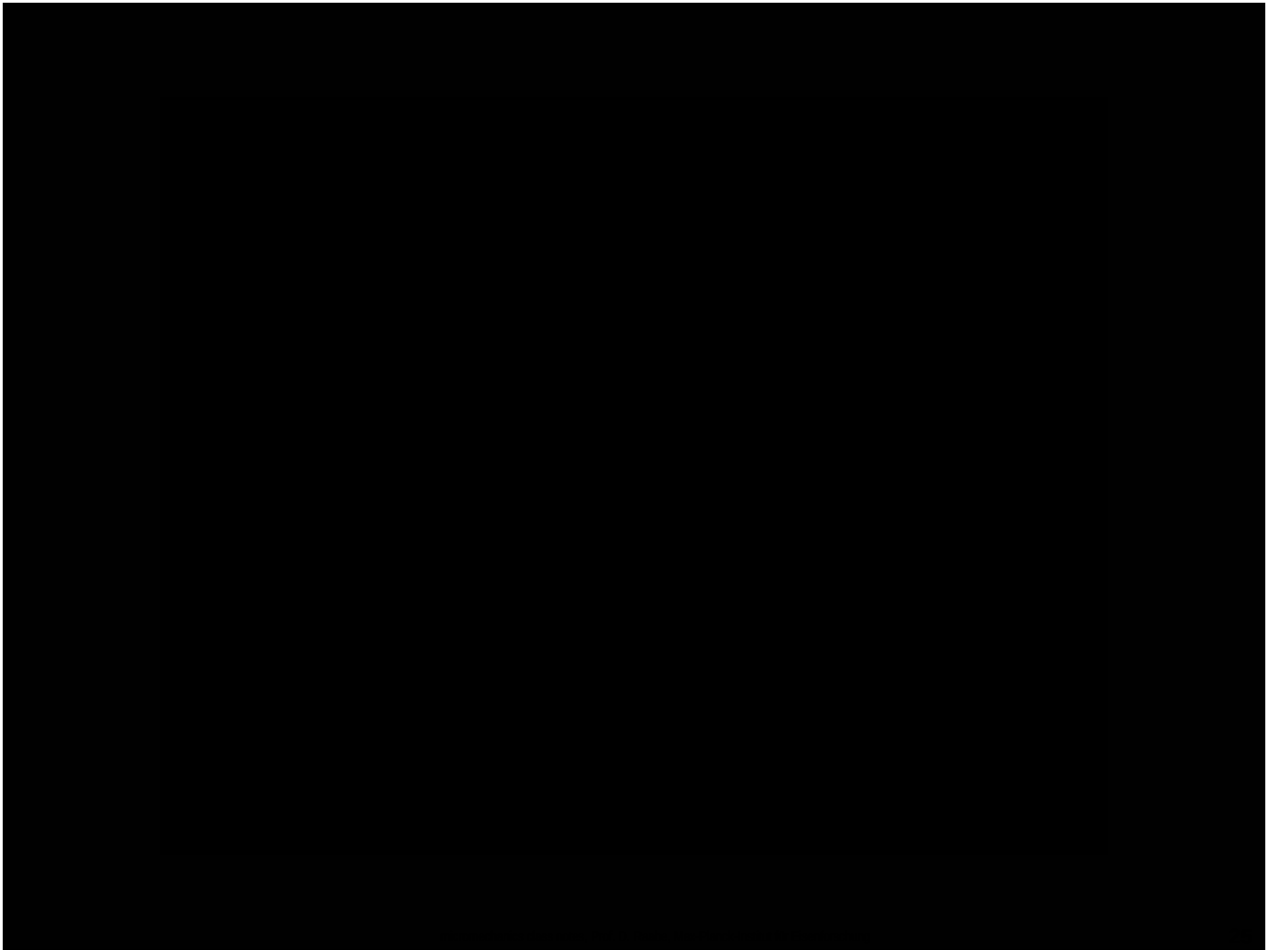


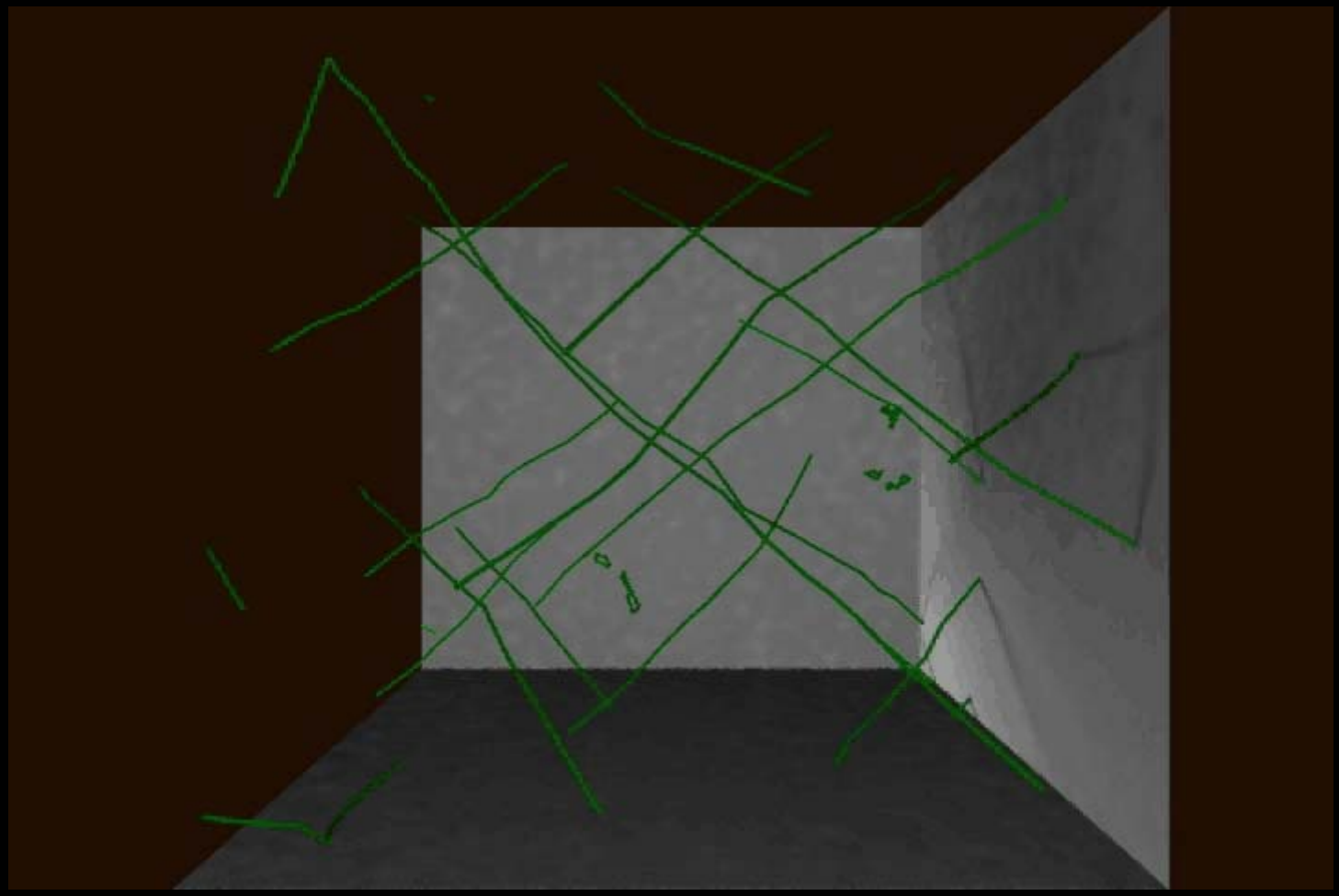
dislocations









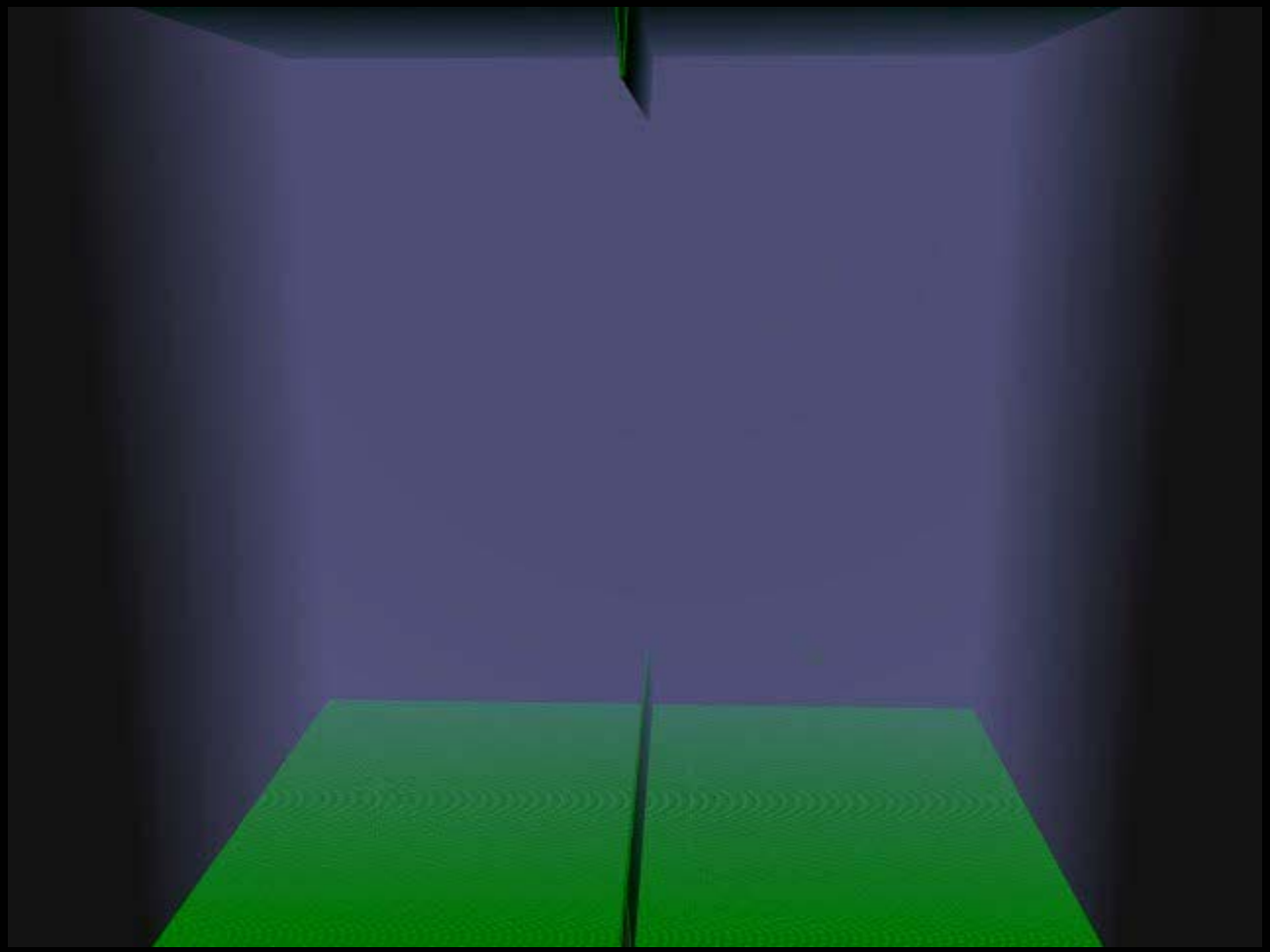


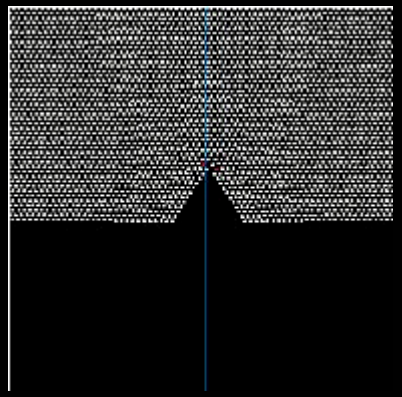
Simulation alternative:

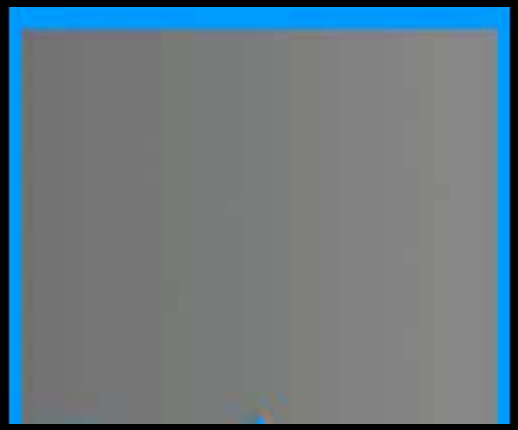
- direct atomistic dynamics (molecular dynamics)

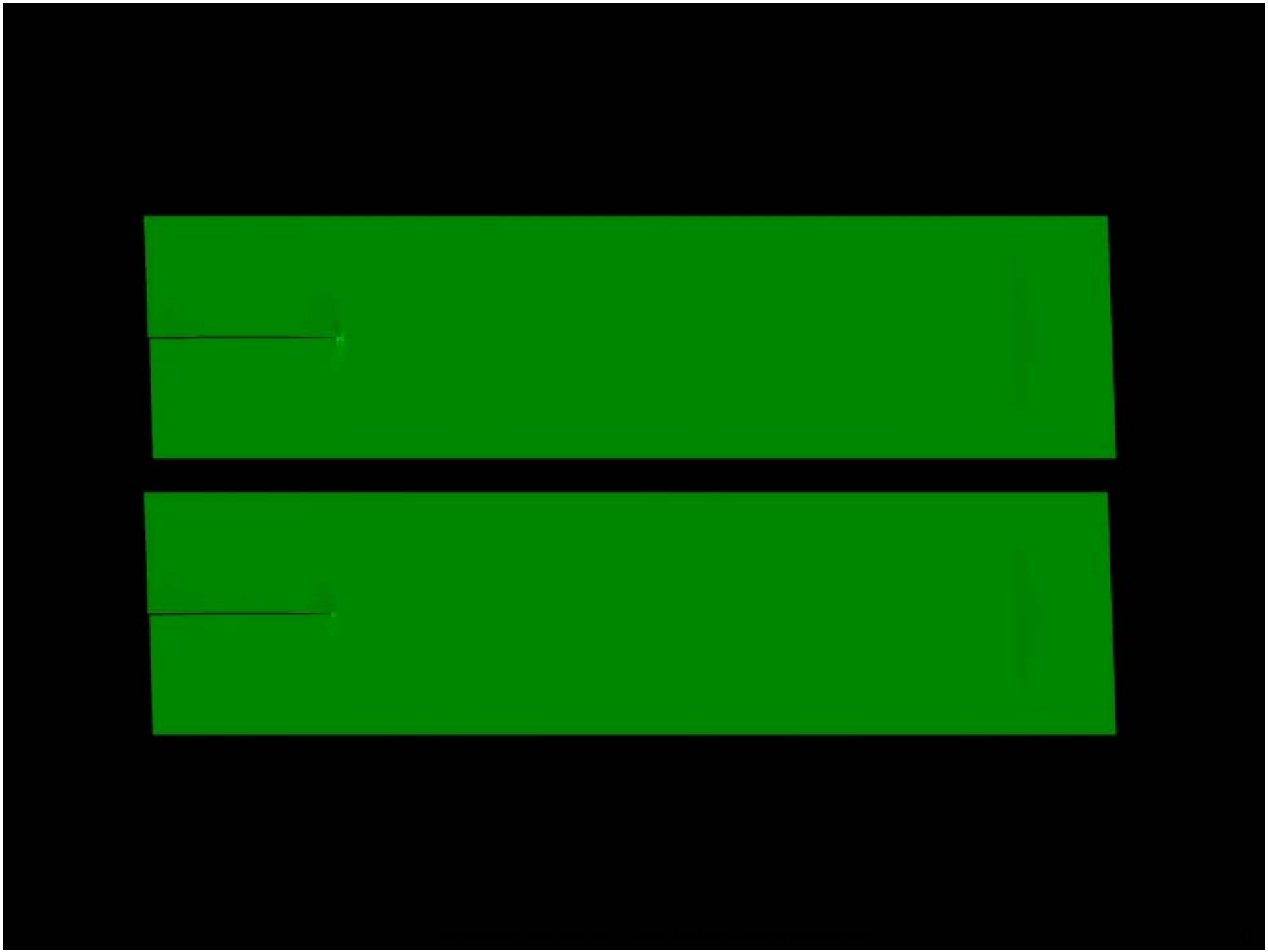
$$F = -\frac{\mathrm{d}U}{\mathrm{d}x}$$

$$F = m\frac{\mathrm{d}\dot{x}}{\mathrm{d}t}$$







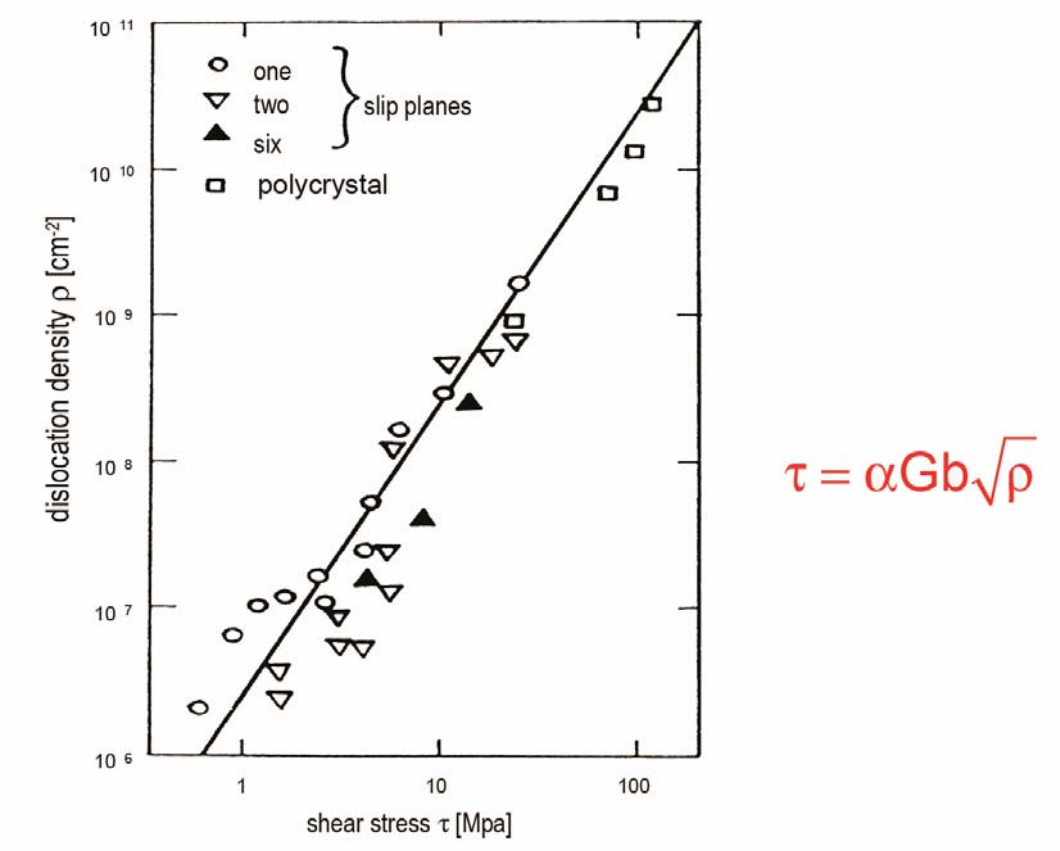


•Statistical Dislocation Dynamics

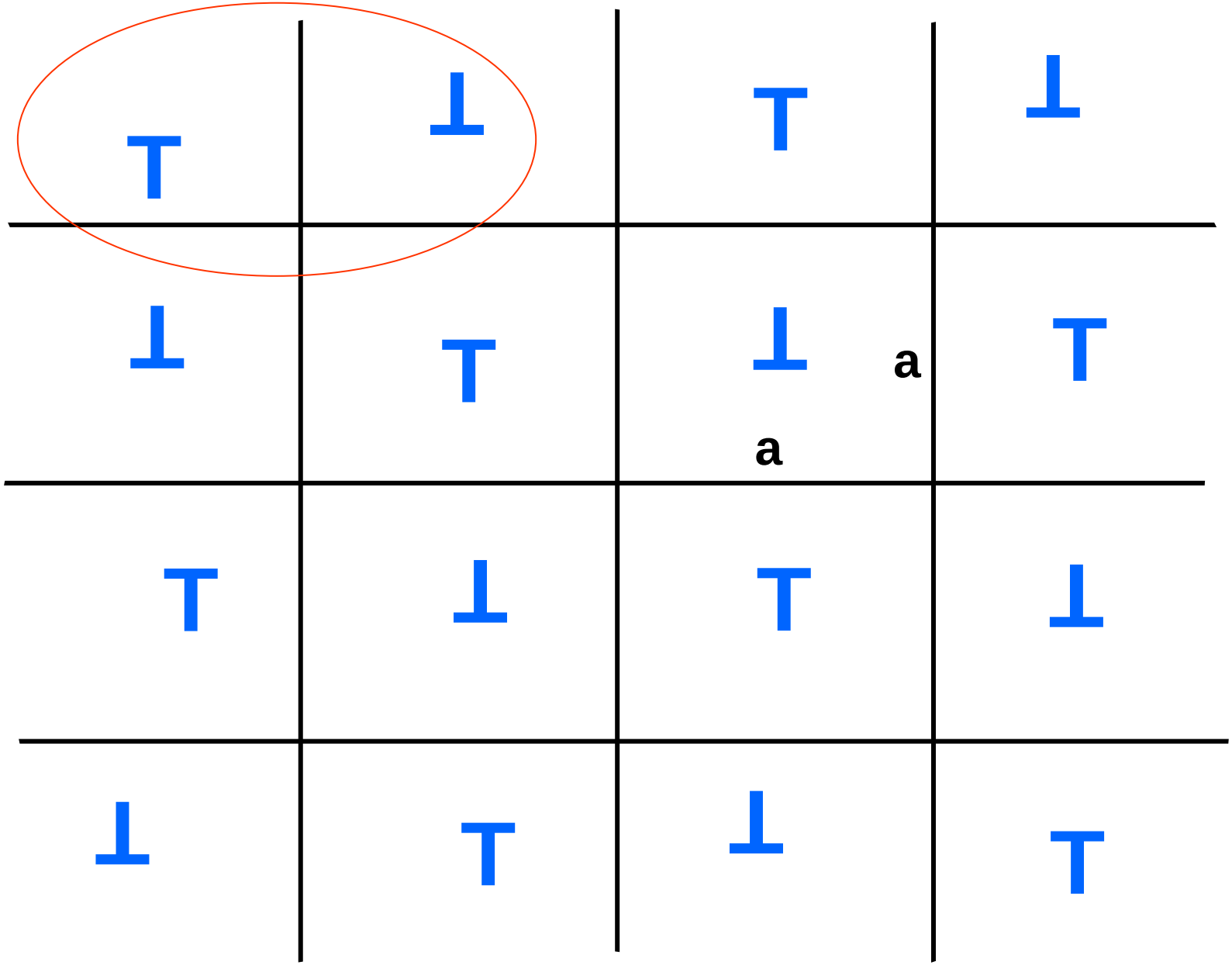
WHY Statistical Dislocation Dynamics ?

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

- kinetic equation of state



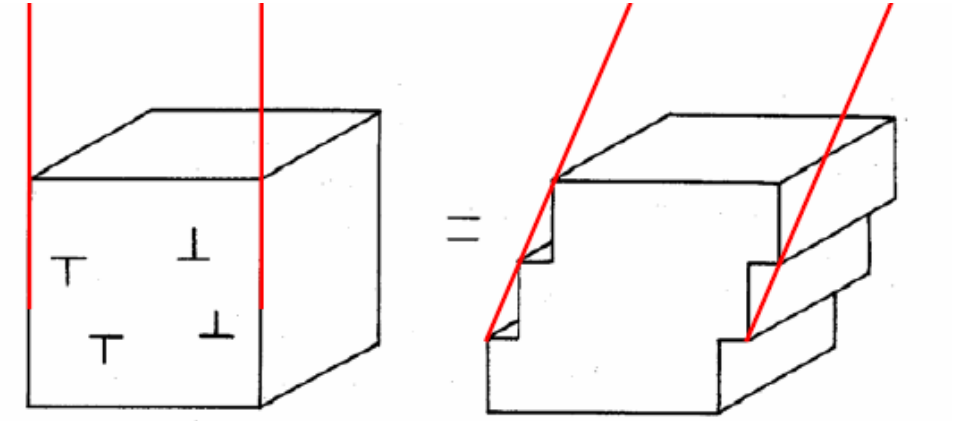
$$\tau = \alpha G b \sqrt{\rho}$$


a
a

- structure evolution

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

- coupling to continuum kinematics



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