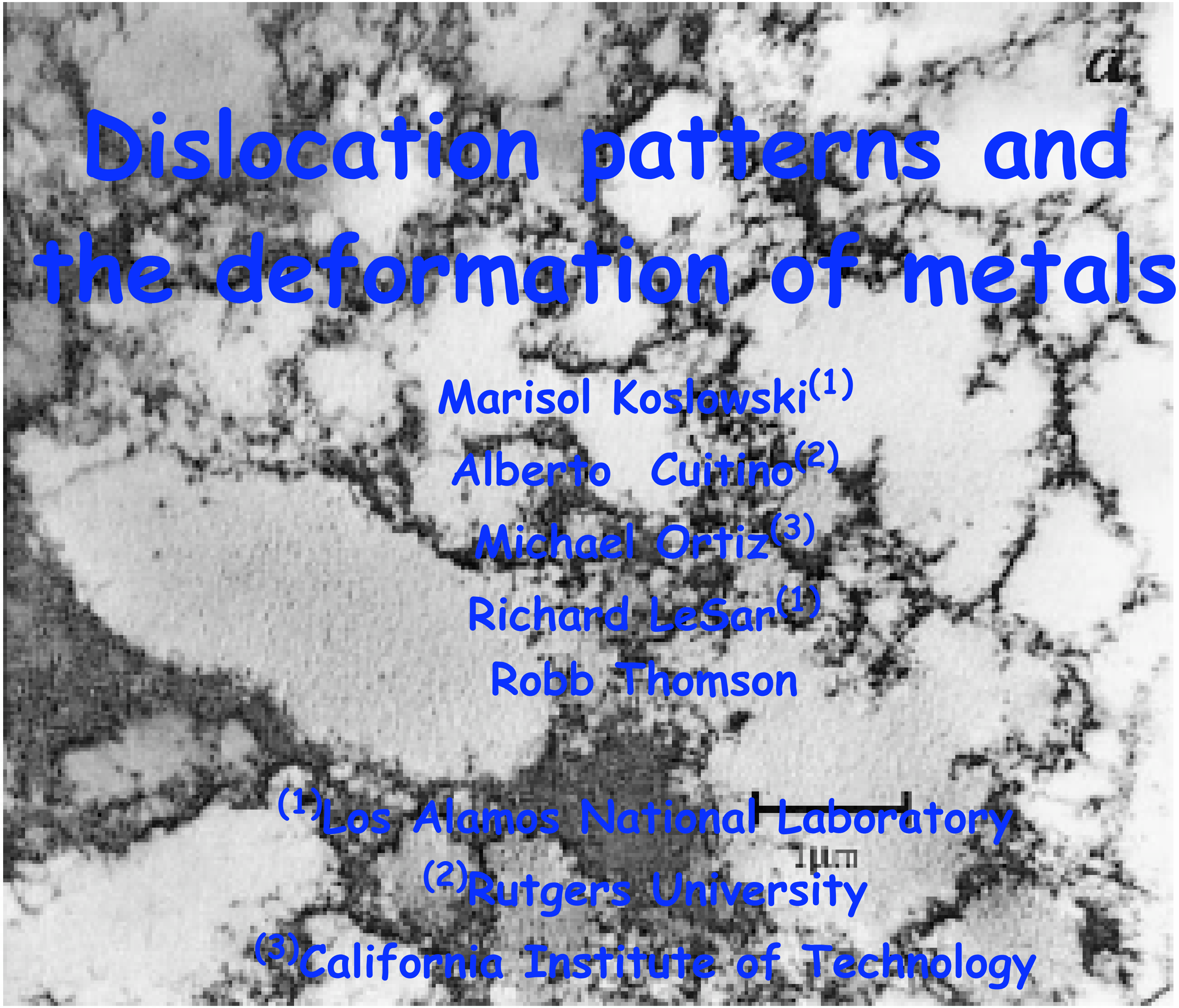

Dislocation patterns and the deformation of metals

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Motivation

- Dislocation patterns are closely coupled to macroscopic response.

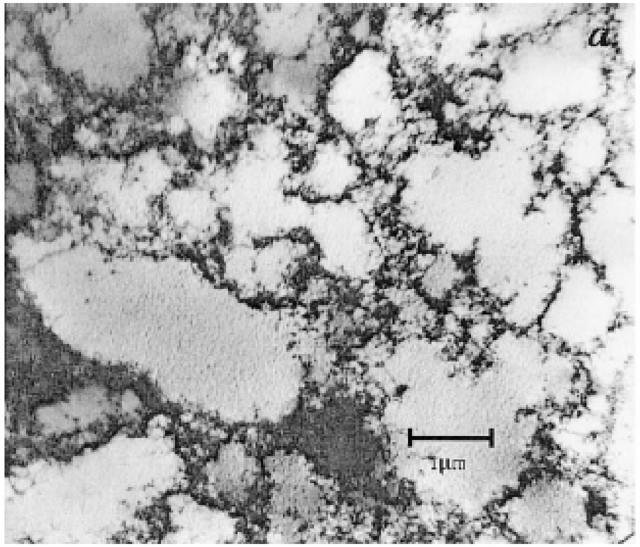
- Stochastic models of stage II/III transition:
    - Noise induced transition.
    - Structures that minimize the energy.

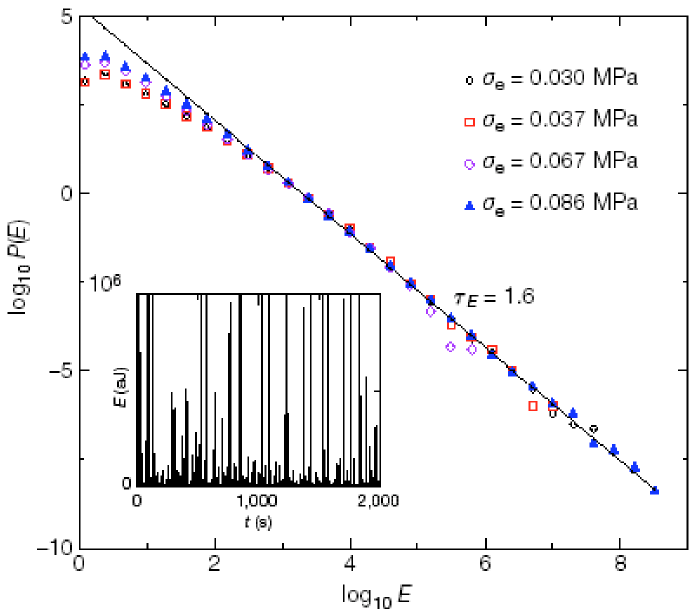
- Characterization of self similar structures:
    - Dislocation density fluctuation.
    - Fractal dimension.

- Intermittent plastic flow.

- Avalanches of dislocations follow a power law behavior.

- Self organized criticality.





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Overview

- Phase-field theory of dislocations.
- Cyclic loading.
- Dislocation networks in twist boundaries.
- We are able to describe the microstructure evolution and the macroscopic response during stage I, II and III.
- The dislocation density fluctuation exhibits a maximum corresponding to the stage II to III transition which is observed in X-ray diffraction experiments (Szekely, Groma, Lendavi, 2002).
- We obtain a stress dependent fractal exponent (Hahner, Bay, Zaiser, 1998).
- Plastic flow is intermittent: avalanches of dislocation motion. (Miguel, 2001, Weiss, 2003)

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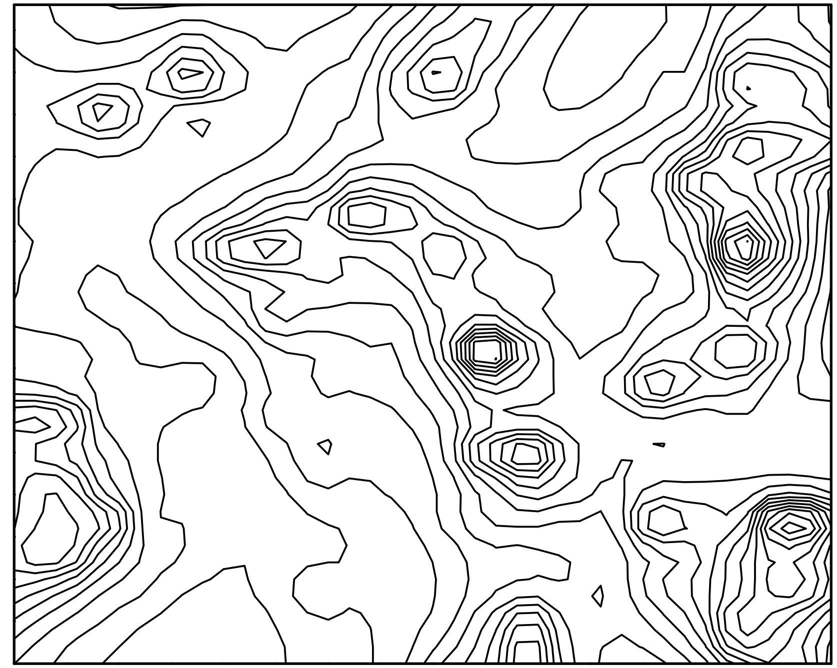
Microstructural evolution in single crystals

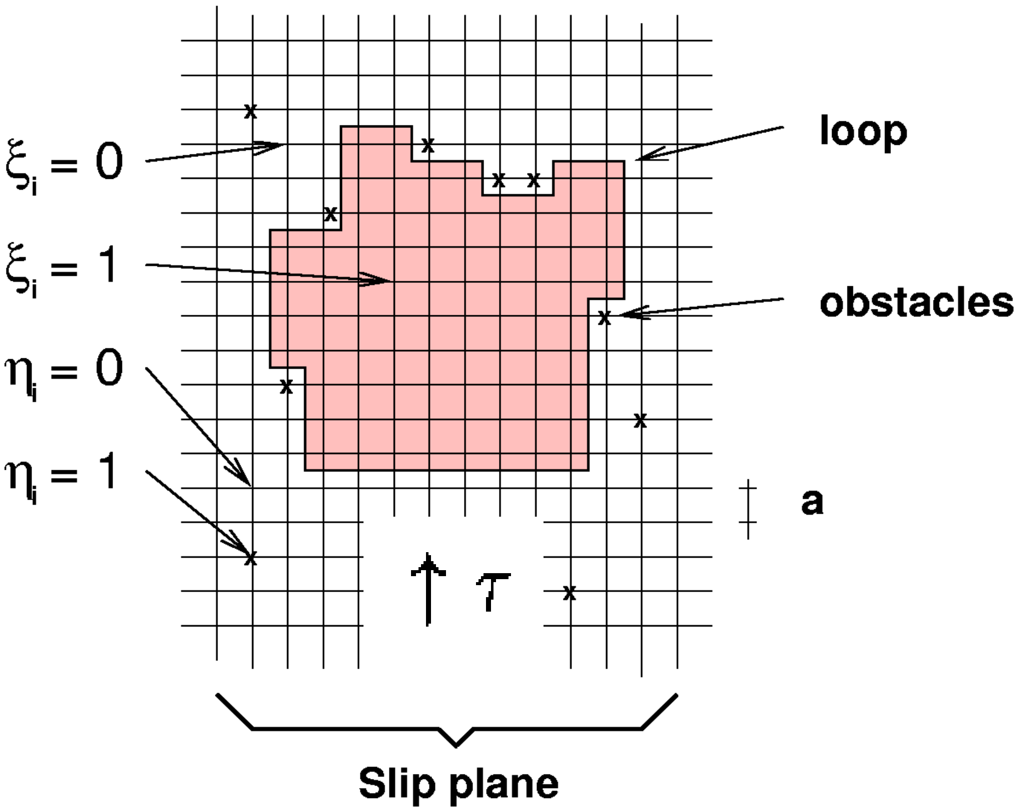


As seen looking down on the slip plane.

Blow up of loops

We approximate 3D by considering dislocations that cross slip plane as obstacles and then model only the 2D expanding loops.

Phase-field model of dislocations



Lattice model of dislocation
loop-point obstacle interaction

Koslowski, Cuitino, Ortiz, 2002

Effective Dislocation Energy

Core Energy

Dislocation Interaction

Irreversible Obstacle Interaction

Equilibrium configurations

Closed form solution at zero temperature.

Macroscopic Averages

$\square \sim < \square >$ $\quad$ $\square \sim < |\square\square| >$

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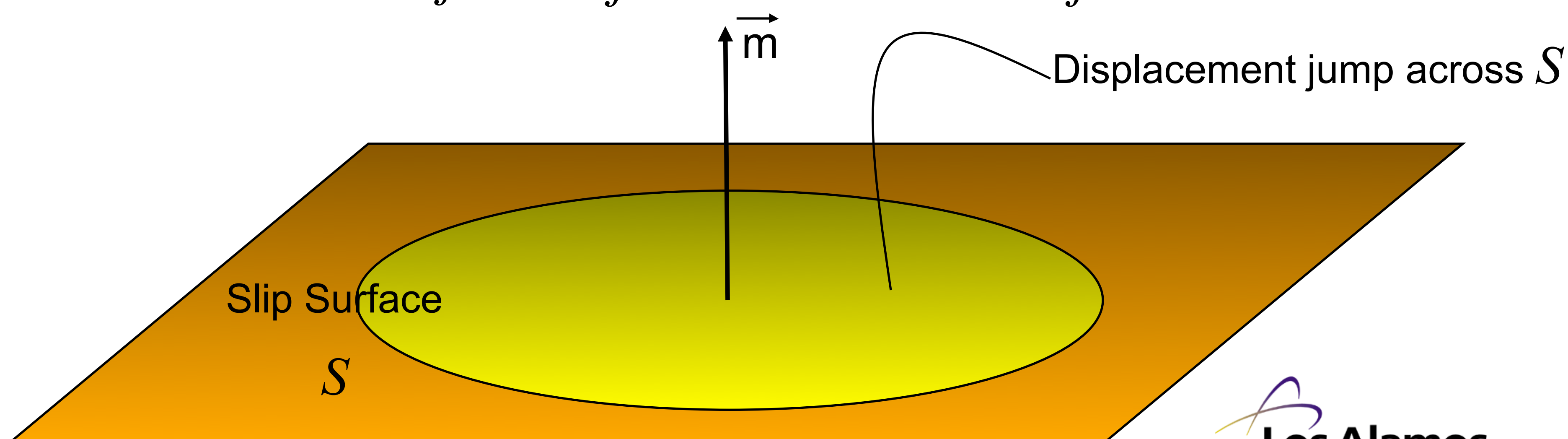
Effective energy

$$E = \int_S \square(\square)\, dS + \int \frac{1}{2} c_{ijkl} \square^e_{ij} \square^e_{kl}\, d^3x - \int_S t_i \square_i\, dS$$

core energy   elastic interaction   applied stress

$$u_{i,j} = \square^e_{ij} + \square^p_{ij} \qquad \square^p_{ij} = b \square_i m_j \square_S$$



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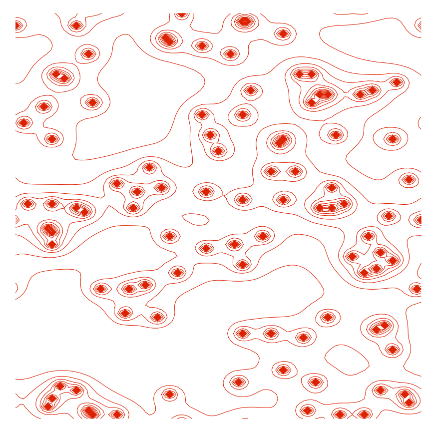
Phase-field energy

$$E[\Box] = E_0 + \frac{1}{(2\Box)^2}\int\left(\frac{\mu b^2}{4}\frac{K}{1+Kd/2}|\hat{\Box}|^2 - \frac{b\hat{s}\hat{\Box}}{1+Kd/2}\right)d^2k$$

with

$$K = \frac{k_2^2}{\sqrt{k_1^2+k_2^2}} + \frac{1}{1-\Box}\frac{k_1^2}{\sqrt{k_1^2+k_2^2}}$$



Closed form solution

$$\frac{\mu b}{2}\hat{\Box} = \hat{s}$$

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Irreversible process and kinetics

Irreversible dislocation-obstacle interaction may be built into a variational framework, we introduce the incremental work function:

$$W[\Box^{n+1}|\Box^{n}] = E[\Box^{n+1}] - E[\Box^{n}] + \int f(x)|\Box^{n+1}(x) - \Box^{n}(x)|d^2x$$

Primary and forest dislocations react to form a jog:

$$f \sim \frac{\mu b}{4\Box}$$

Updated phase-field follows from:

$$\min_{\Box^{n+1}\in Y} W[\Box^{n+1}|\Box^{n}]$$

Short range obstacles:

$$f(x) = b\Box^{P} + \Box_{i=1}^{N} f_i \Box_d(x - x_i)$$

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Irreversible process and kinetics

$$\int f(x)\,|\square^{n+1}(x)-\square^{n}(x)|\,d^2x = \sup_{|g^{n+1}|\le f} \int g^{n+1}(x)\big(\square^{n+1}(x)-\square^{n}(x)\big)\,d^2x$$

Kuhn-Tucker optimality conditions $\quad \square^{n+1}(x)-\square^{n}(x)=\square^{+}(x)-\square^{-}(x)$

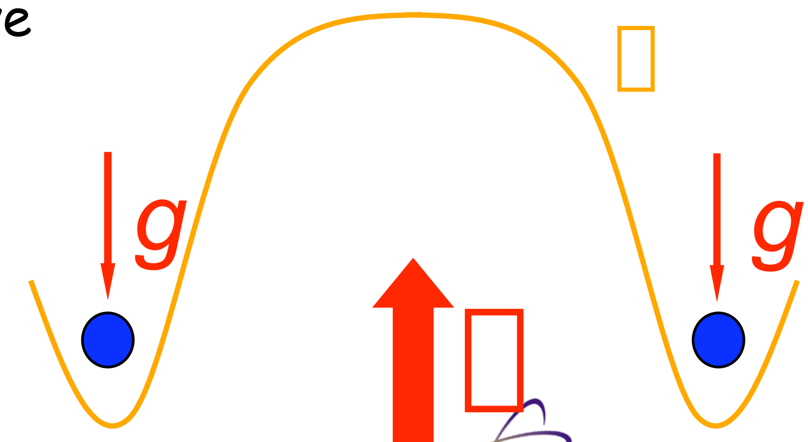
$$\mathrm{g}^{n+1}(x)-f(x)\le 0 \qquad -\mathrm{g}^{n+1}(x)-f(x)\le 0$$

$$\square^{+}(x)\ge 0,\quad \square^{-}(x)\ge 0$$

$$\big(g^{n+1}(x)-f(x)\big)\square^{+}(x)=0,\quad \big(g^{n+1}(x)+f(x)\big)\square^{-}(x)=0$$

Equilibrium condition: Fredholm alternative

$$\int b\,s_{n+1}(x)\,d^2x=\int g^{n+1}(x)\,d^2x$$



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Macroscopic averages

Slip $$\square = \frac{\square_0}{|\square|}\int_{\square} \square \, d^2x = \square_0 \langle \square \rangle$$

with $$\square_0 = \frac{b}{l}$$

Dislocation density $$\square = \frac{1}{l}\langle | \square \square | \rangle$$

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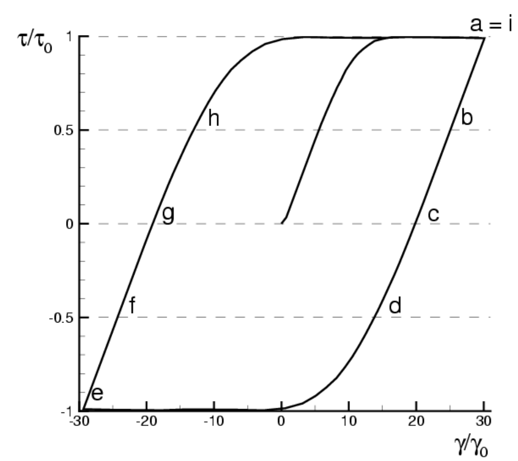
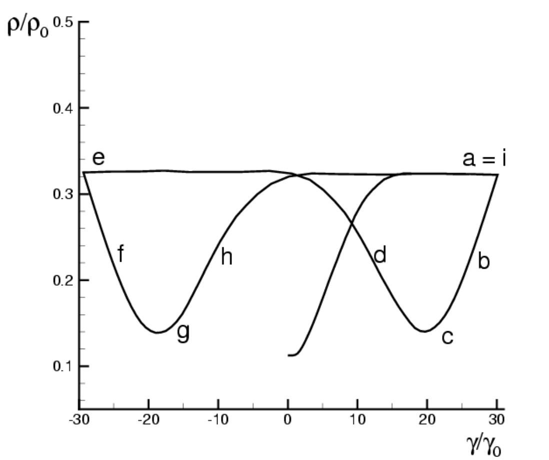
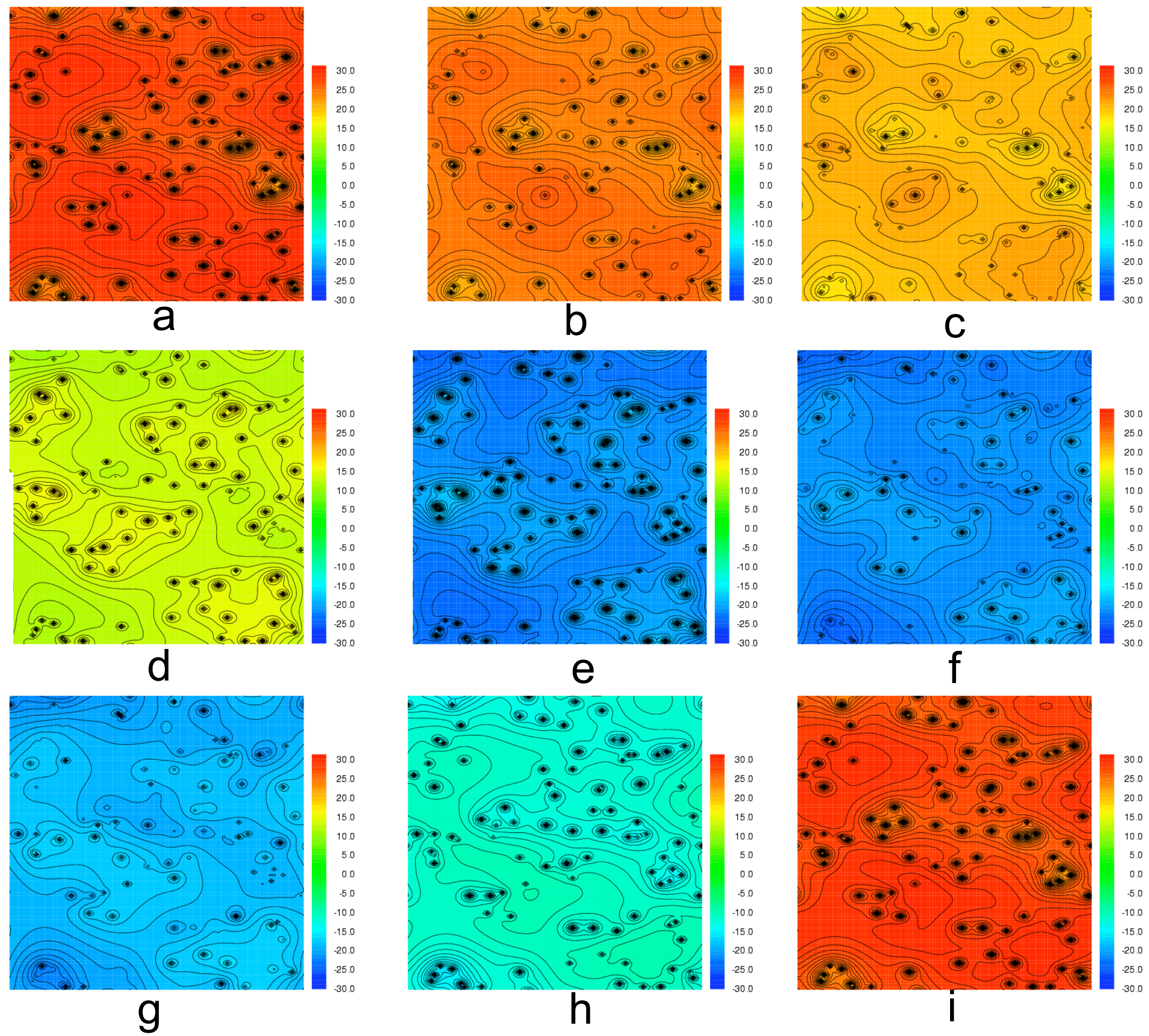
Single-slip



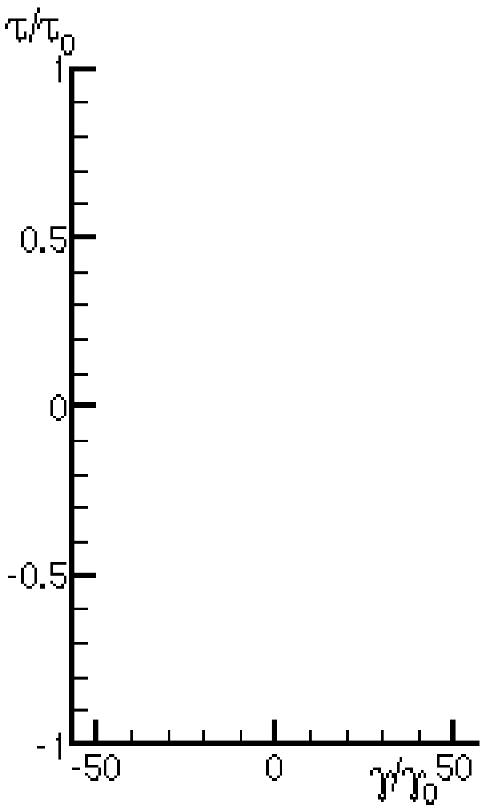
Stress-strain curve.



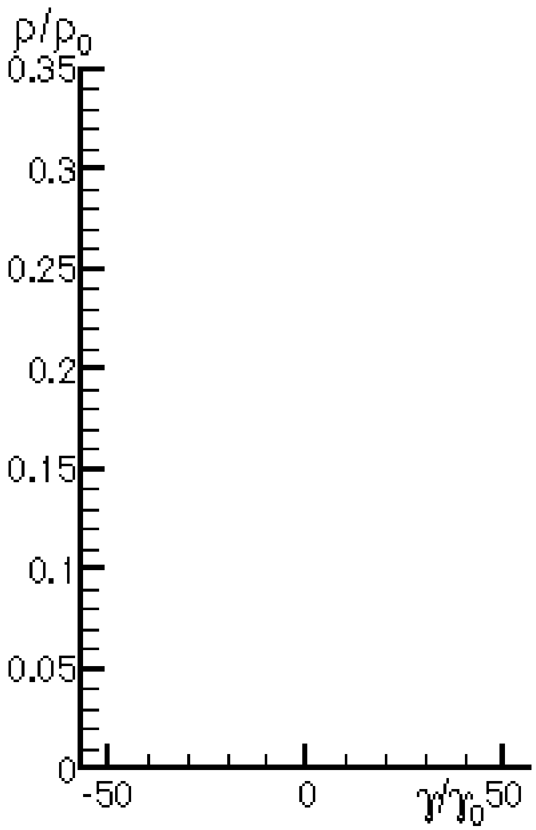
Evolution of dislocation density with strain.



Cyclic loading



Stress-strain curve.



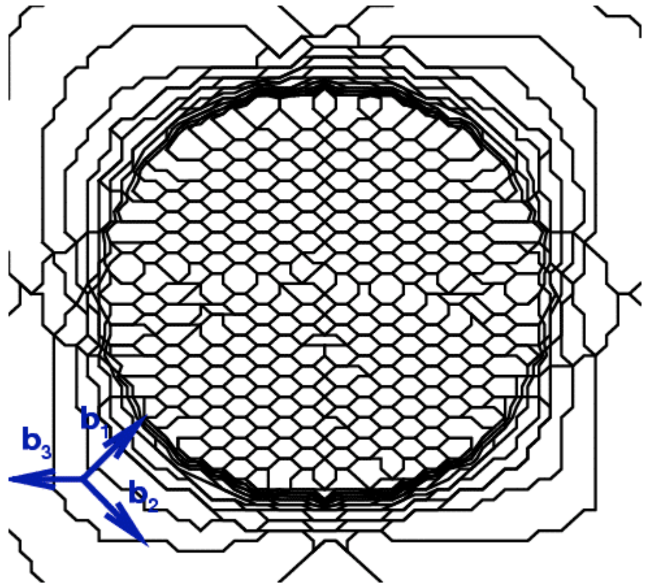
Evolution of dislocation density with strain.

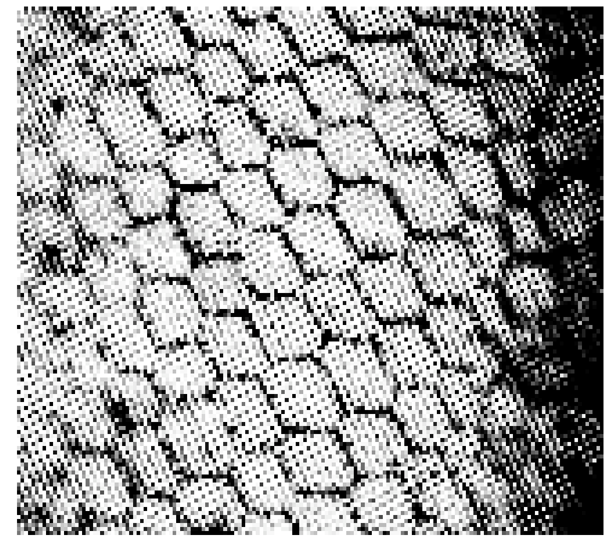
Dislocation networks in twist boundaries

When the rotation axis is the [111] the grain boundary is a hexagonal grid of screw dislocations with Burgers vectors:

$$b_1 = \tfrac{1}{2}[1,1,0] \quad b_2 = \tfrac{1}{2}[1,0,1]$$

$$b_3 = \tfrac{1}{2}[0,1,1]$$

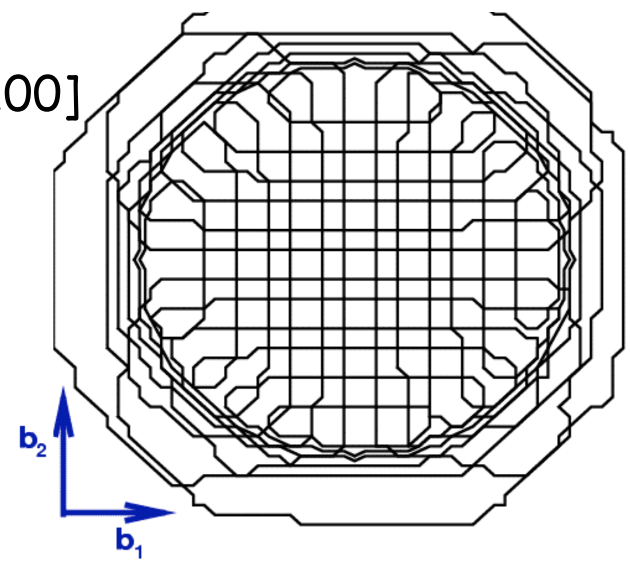


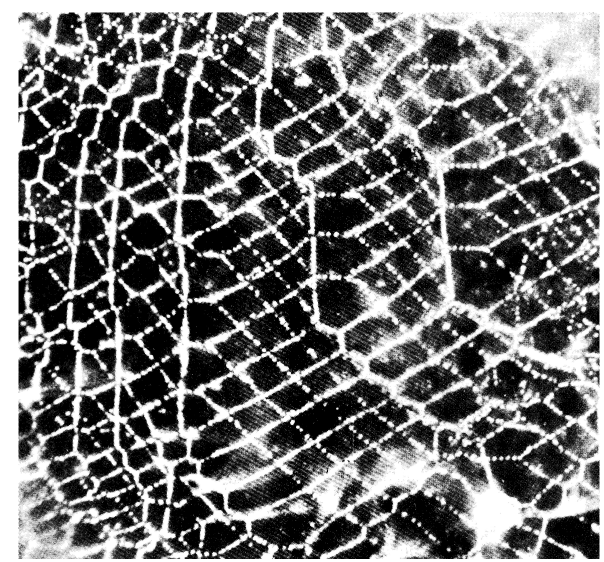


A twist boundary having a [100] rotation axis consists of a square grid of screw dislocations with Burgers vectors:

$$b_1 = \tfrac{1}{2}[0,1,1]$$

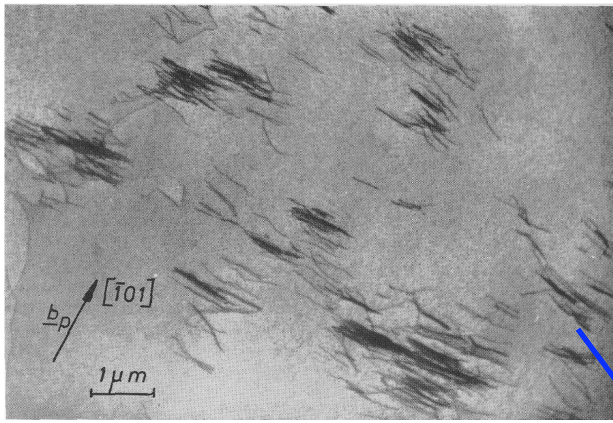
$$b_2 = \tfrac{1}{2}[0,1,-1]$$



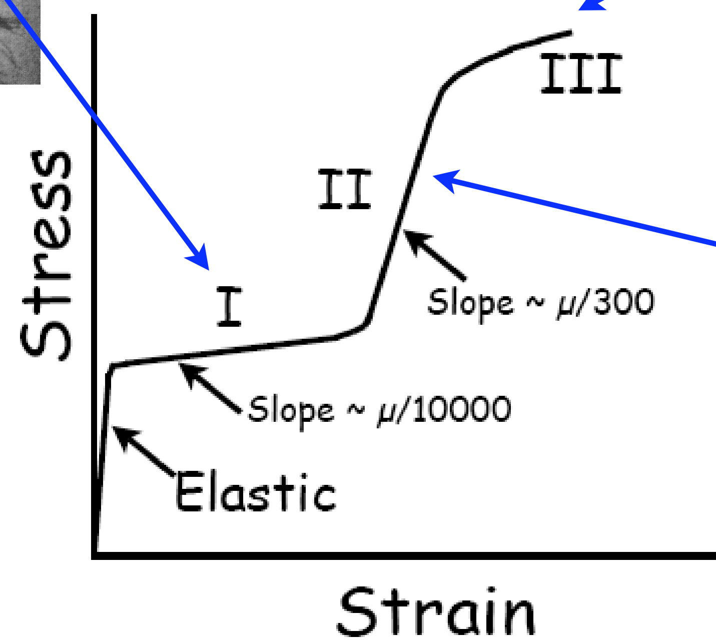


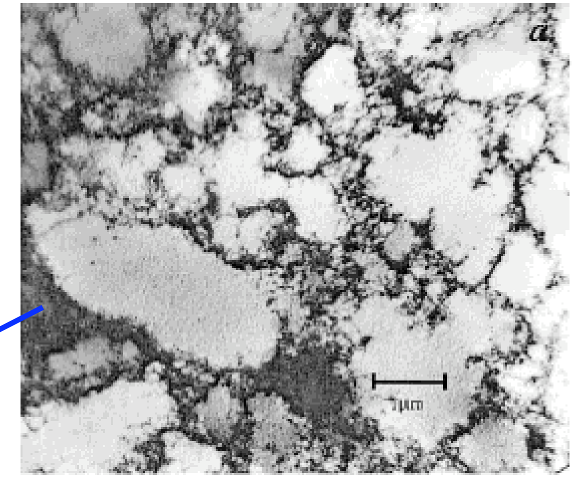
S. Amelinckx, 1958

Structure and response are closely coupled.

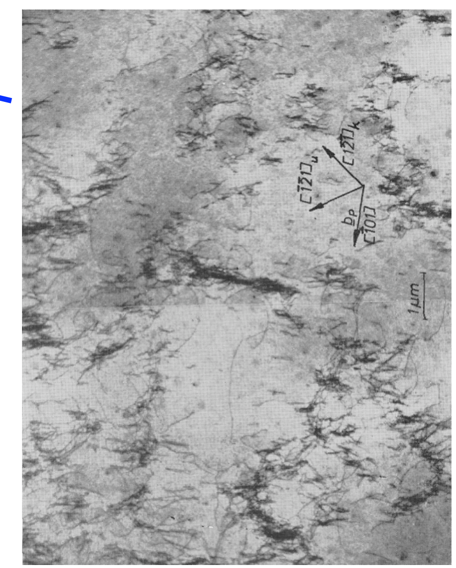


Mughrabi, Phil. Mag. **23**, 869 (1971)





Szekely, Groma, Lendvai, Mat. Sci. Engin. A **324**, 179 (2002)



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

Hardening regimes show very different microstructures.

All micrographs from a Cu single crystal

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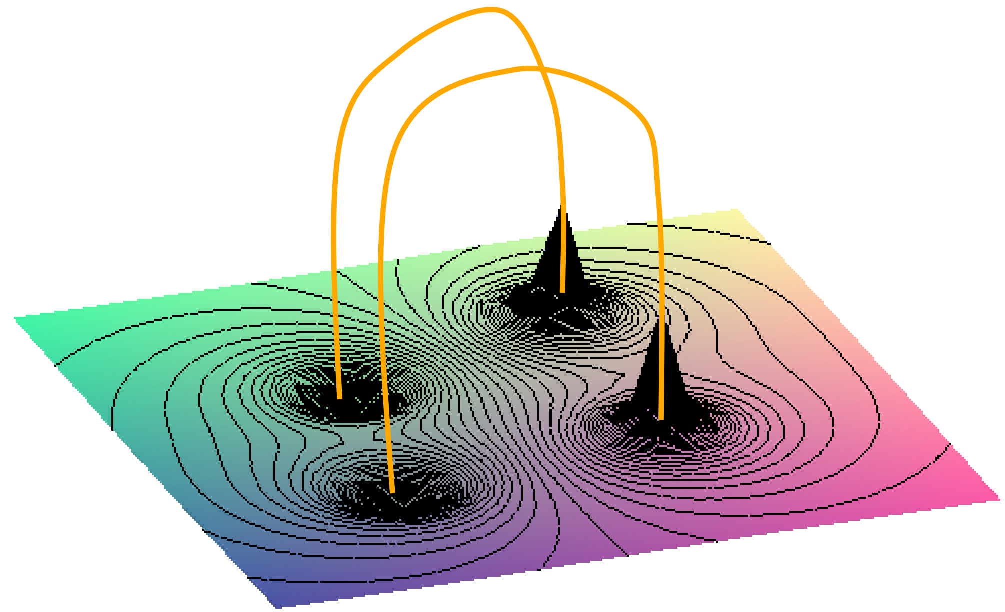
Forest hardening

- At the onset of stage II other slip systems become active.

- The number of forest dislocations in the slip plane follows Taylor's hardening law:

$$\tau \sim \mu b\sqrt{\rho}$$



Forest dislocations piercing the slip plane.

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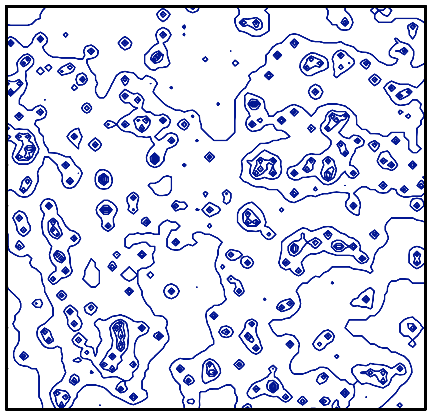
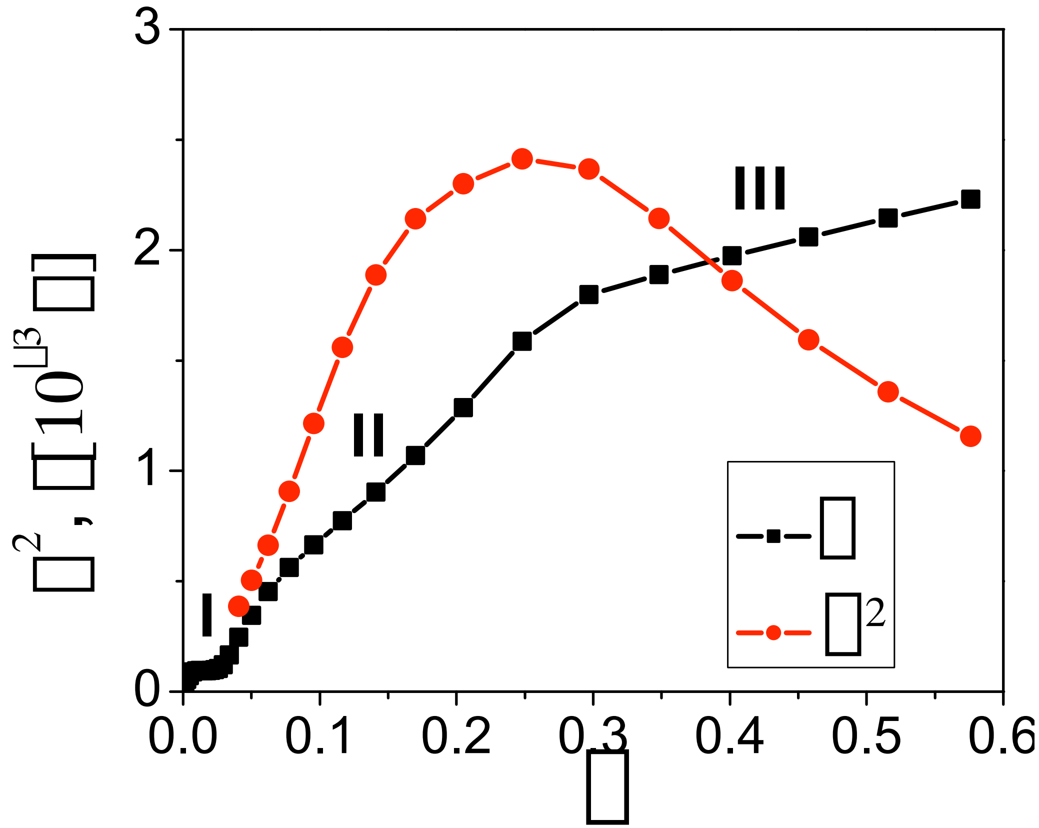
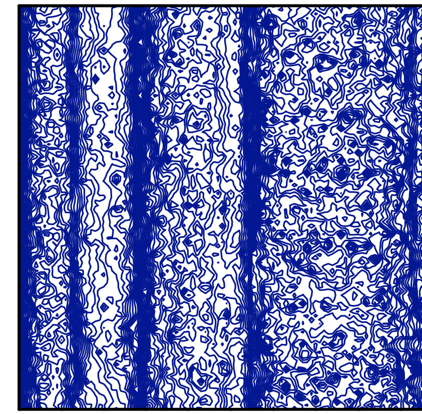
Model predictions of structure and response

Hardening regimes show very different microstructures.

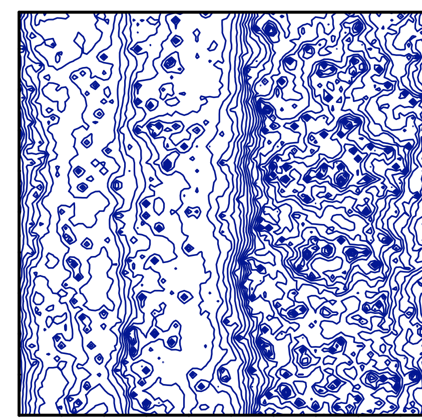


Stage I





Stage III



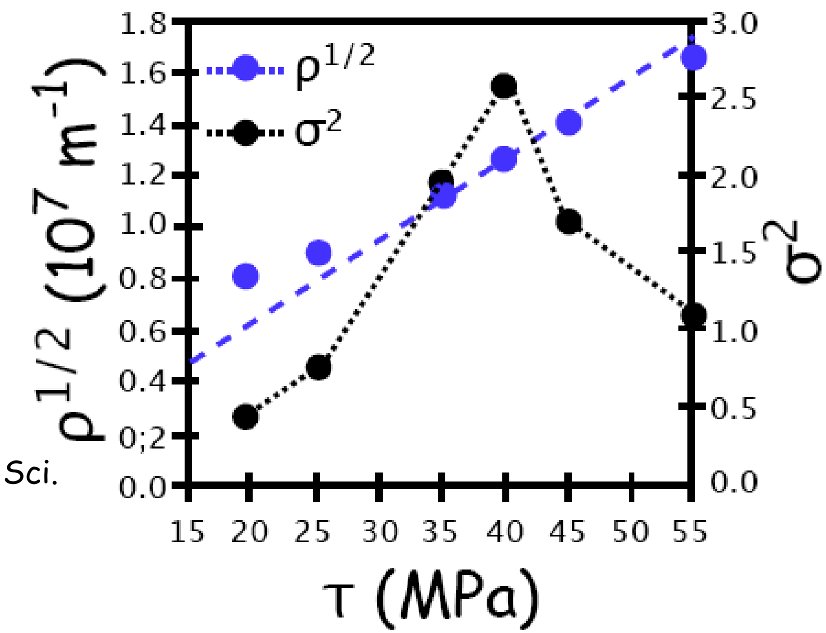
Stage II

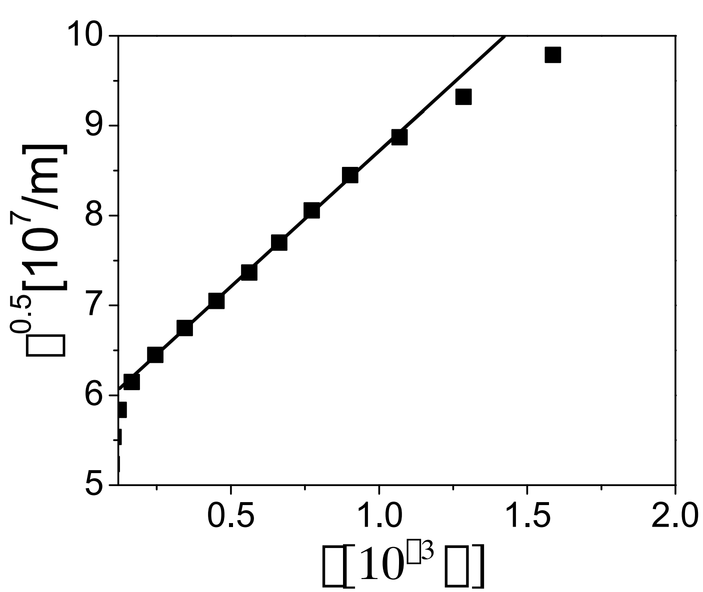
2D obstacle model shows correct behavior of dislocation density across the stages

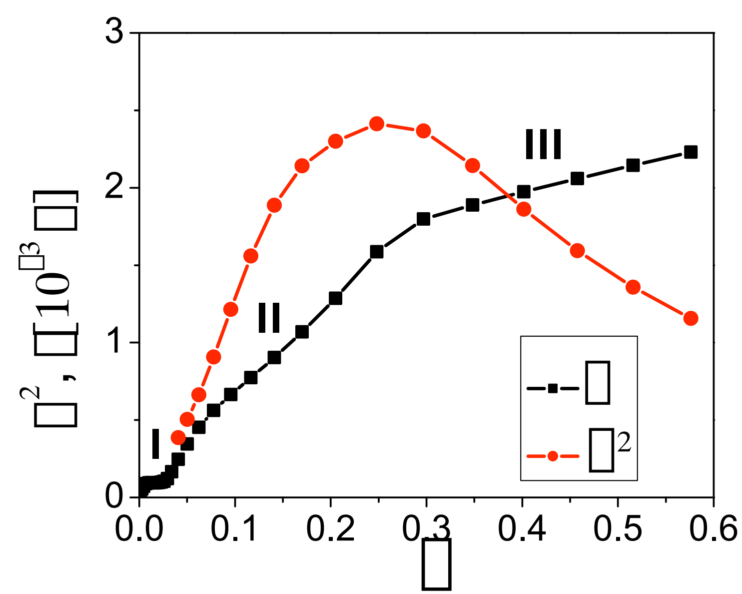
Dislocation density fluctuation has a maximum at stage II-III transition.

$$\sigma^2 = \frac{\langle \rho^2 \rangle - \langle \rho \rangle^2}{\langle \rho \rangle^2}$$

Szekely, Groma, Lendvai, Mat. Sci. Engin. A **324**, 179 (2002)







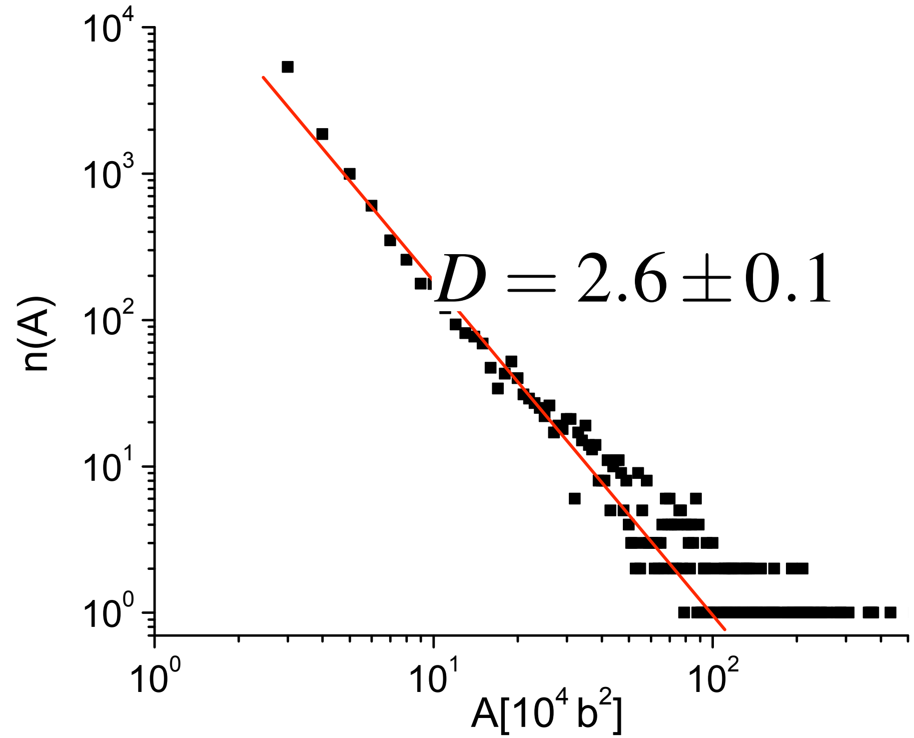
Characterization of self-similar cell structures

The cell size distribution has an hyperbolic frequency:

$$n(A) = CA^{-D}$$

Formation of cell structures corresponds to the regimen

$$2 < D < 3$$



applied stress: $\square = 1.1 \cdot 10^{-3} \mu$

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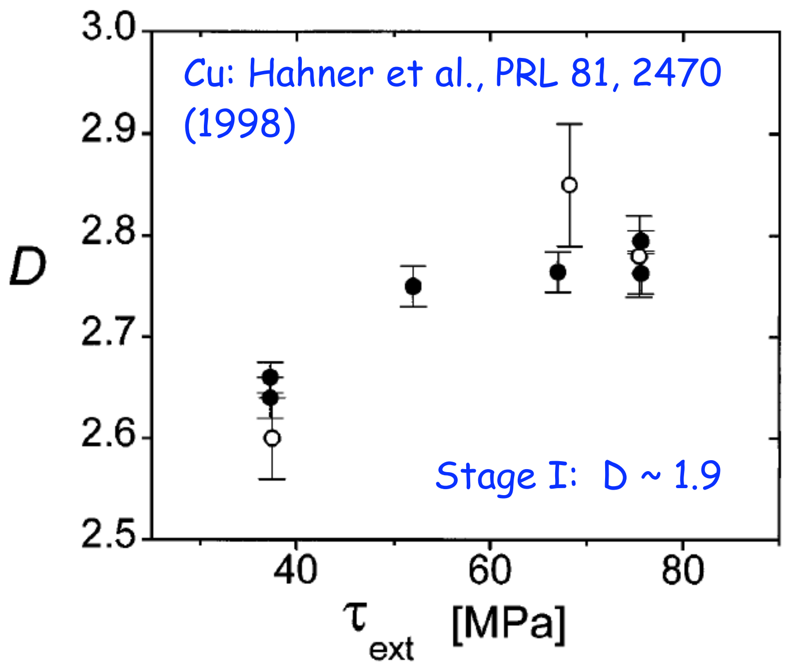
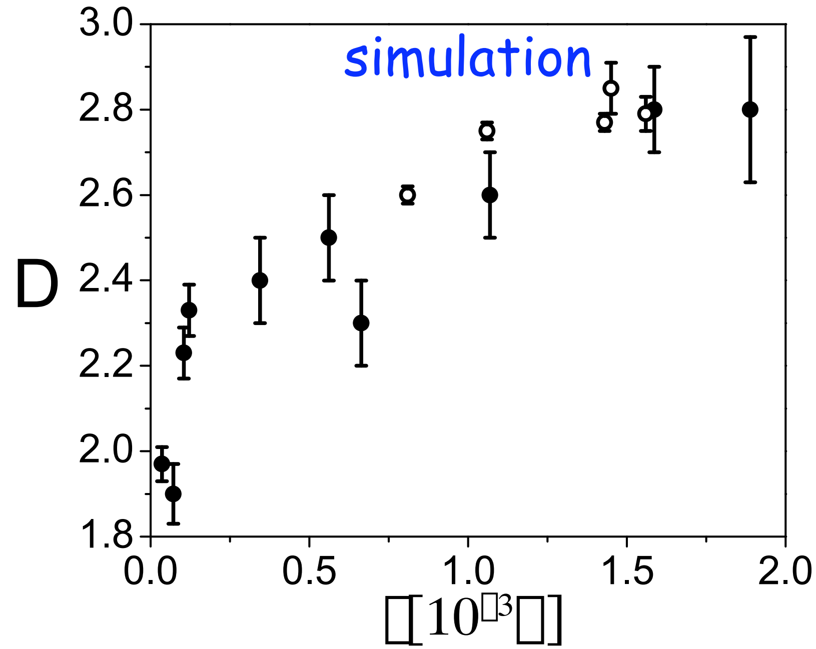
Self-similar structures

Dislocation patterning is **fractal**

- first discussed by Gil Sevillano and shown in Cu by Hahner
- probability of cells of size A $n(A) \sim A^{-D}$
  - D is the fractal dimension.





The 2D model shows excellent agreement with experiment, from stress-strain to density to fractal dimension of structures.

First calculation to show this range of behavior.

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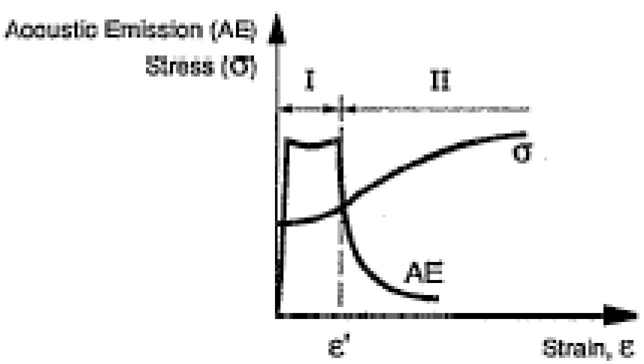
Acoustic emission during plastic flow in ductile single crystals

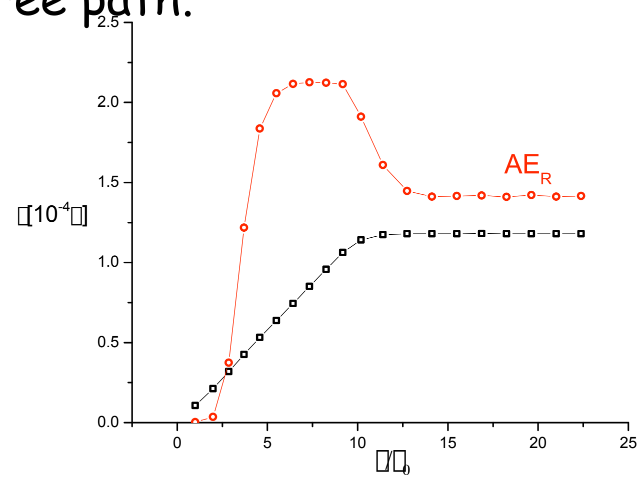
• The motion of great number of dislocations are 'events' that can be detected by acoustic emission (AE) with suitable transducers.

• In single loading experiments on copper single crystals the AE signal rise during the onset of easy glide and decreases after the material yields.

• Even when the dislocation density increases the AE decreases, this reduction is attributed to a the decrease in the dislocation free path.



Stress and acoustic emission in aluminum alloy.



Predictions of stress and acoustic emission during stage I.

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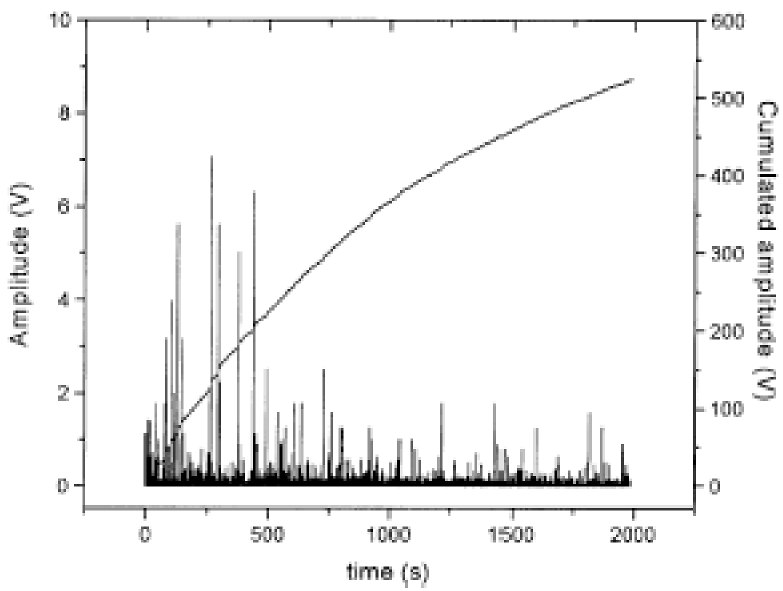
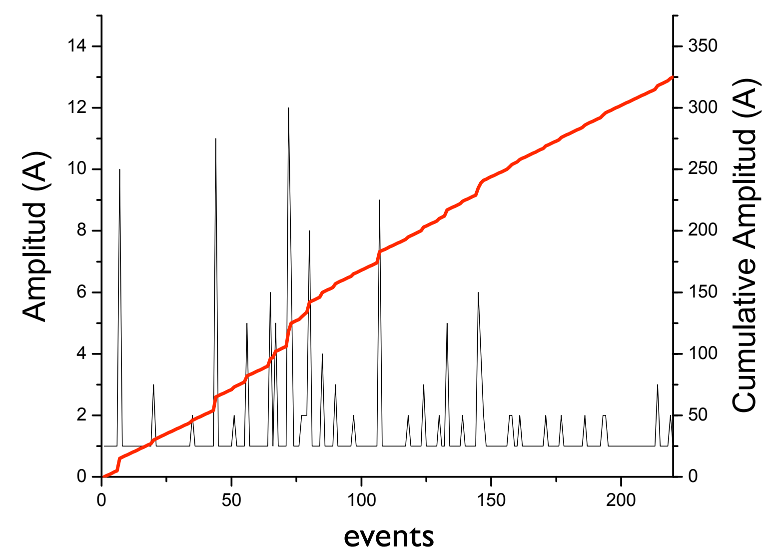
Intermittent dislocation flow in plastic deformation

- The AE signal accompanying the plastic deformation consists of many overlapping pulses as observed experimentally in metallic single crystals (Vinogradov, 2001) and ice single crystals (Weiss, 1997).
- The instantaneous dissipation shows burst of activity that can be considered as dislocation avalanches.
- The cumulated activity is a measure of the strain and and also shows the burst character observed in plastic deformation.(Pond,1973 and Neuhauser, 1983)



Instantaneous and cumulated acoustic activity during a loading step in a compression test (Weiss, 1997)



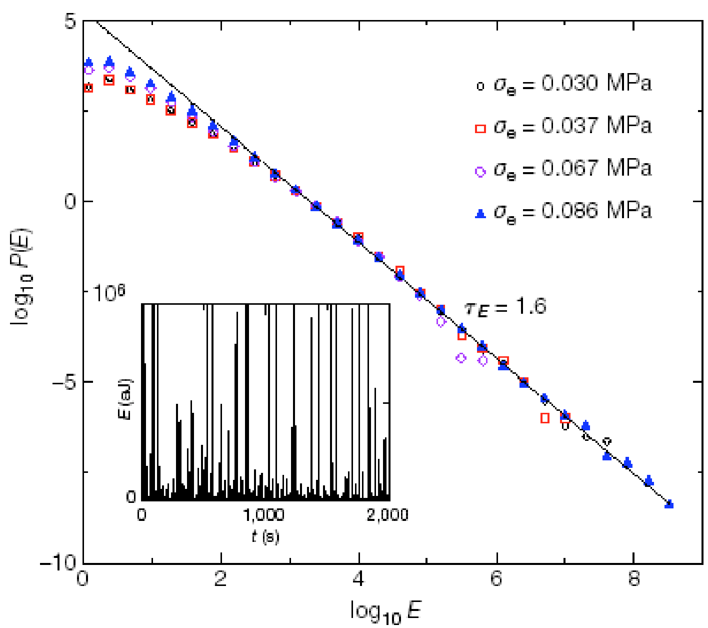
Predicted acoustic activity during a loading step.

Scale-free dislocation avalanches

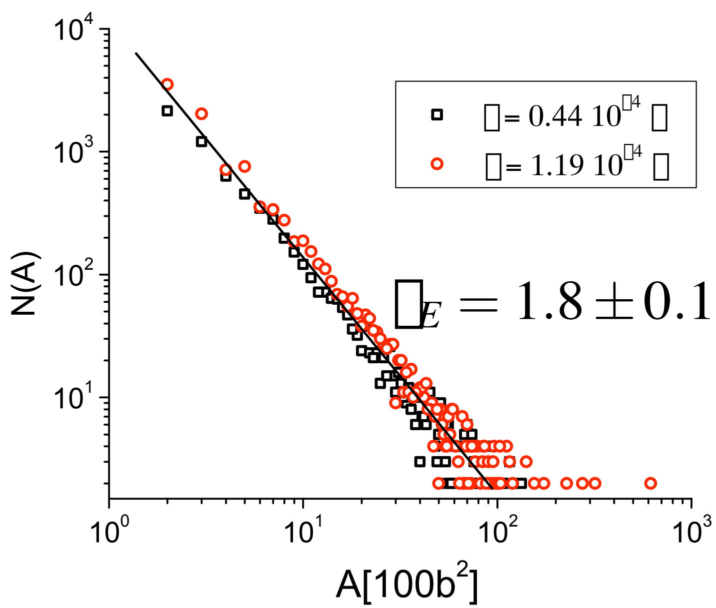
• Recently, acoustic emission experiments on single crystals of ice showed an intermittent and heterogeneous plastic flow.

• The probability density function of the energy, follows a power law distribution

$$P(E) \sim E^{-\tau_E}$$



Statistical properties of acoustic energy bursts under constant stress (Miguel, 2001)



Simulated acoustic energy bursts under constant stress.

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Summary

- The phase-field theory of dislocations allows to investigate the whole range of deformation in ductile single crystals.
- The theory is exactly solvable.
- The model is capable to reproduce experiments:
  - Recovery at the onset of stage III
  - Maximum on the fluctuation of dislocation density during the stage II/III transition.
  - Stress dependent fractal exponent.
  - Properties related to AE experiments.
- The change between stage II and stage III arises from the transition between random and ordered structures. Annihilation is the primary process that drives this transition.
- Characteristics of SOC:
  - Structures are marginally-stable .
  - Slow external driving (creep).
  - Power law distributions.
  - Very large number of interacting entities.

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(2) Multi-phase field model of planar dislocation networks, Koslowski and Ortiz, submitted to **MSMSE,2003.**

(3) A noise induced transition in the deformation of metals, Thomson, Koslowski and LeSar, submitted to **Physica A,2004**

(4) Dislocation structures and the deformation of metals, Koslowski, LeSar and Thomson, to be submitted to **Science, 2004.**

(5) Non-homogeneous plastic flow in single crystals, Koslowski and LeSar, in preparation.

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