Collective Dislocation Phenomena in Non-equilibrium Systems

M.-Carmen Miguel

University of Barcelona

Paolo Moretti, Jérôme Weiss,

Michael Zaiser, Stefano Zapperi

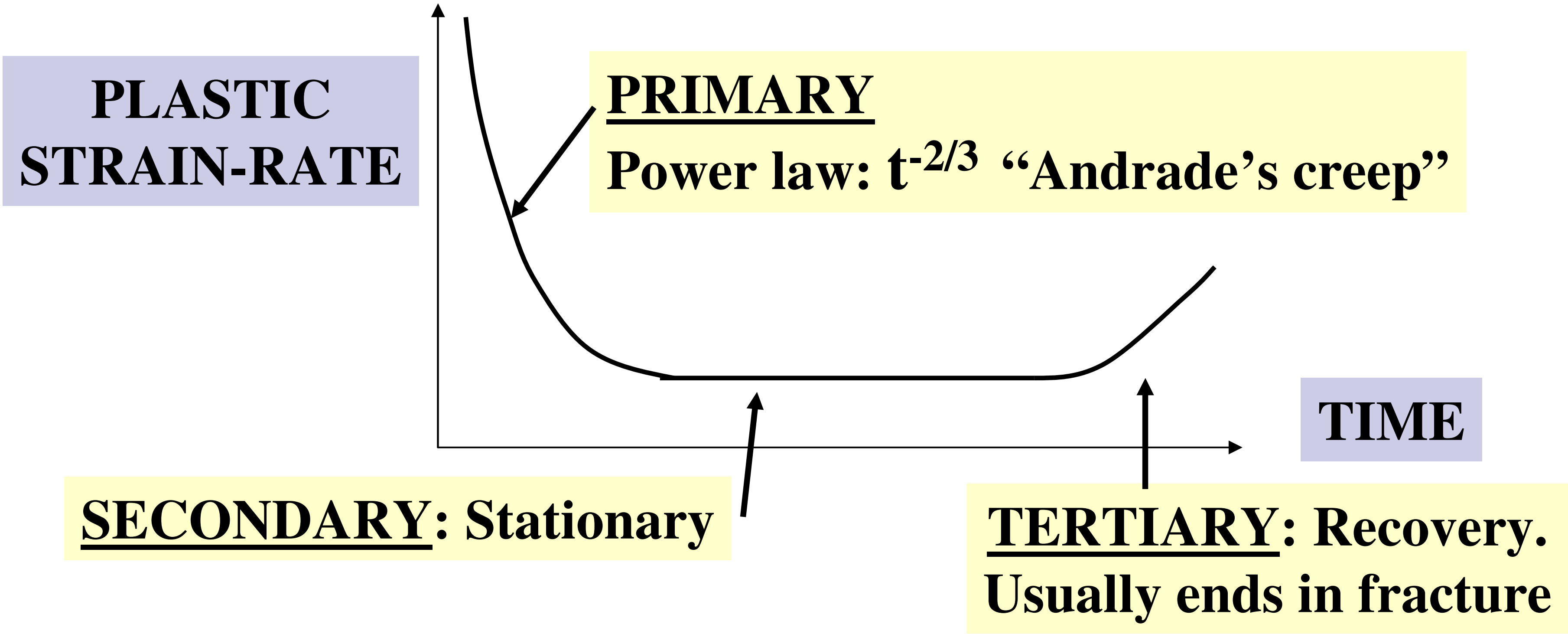
Outline

- Plastic deformation of crystals
  - ***Plastic avalanches*** in ice single crystals
  - Plastic avalanches in 2D dislocation dynamics models
  - Statistical properties under constant stress (creep tests)
  - Dislocation ***jamming transition***
  - ***Aging*** like phenomena
- Slip heterogeneity & surface morphology
  - On microscopic scales …
- The vortex lattice in thin superconducting films: Dislocation dynamics & Plastic flow in quasi-2D
  - Vortex polycrystals: Columnar ***grain growth***
  - Quenched disorder—***Grain boundary pinning/depinning***
  - Experimental data
  - Numerical results: critical current, hysteresis—Metastability
- Conclusions

Time laws of plastic creep

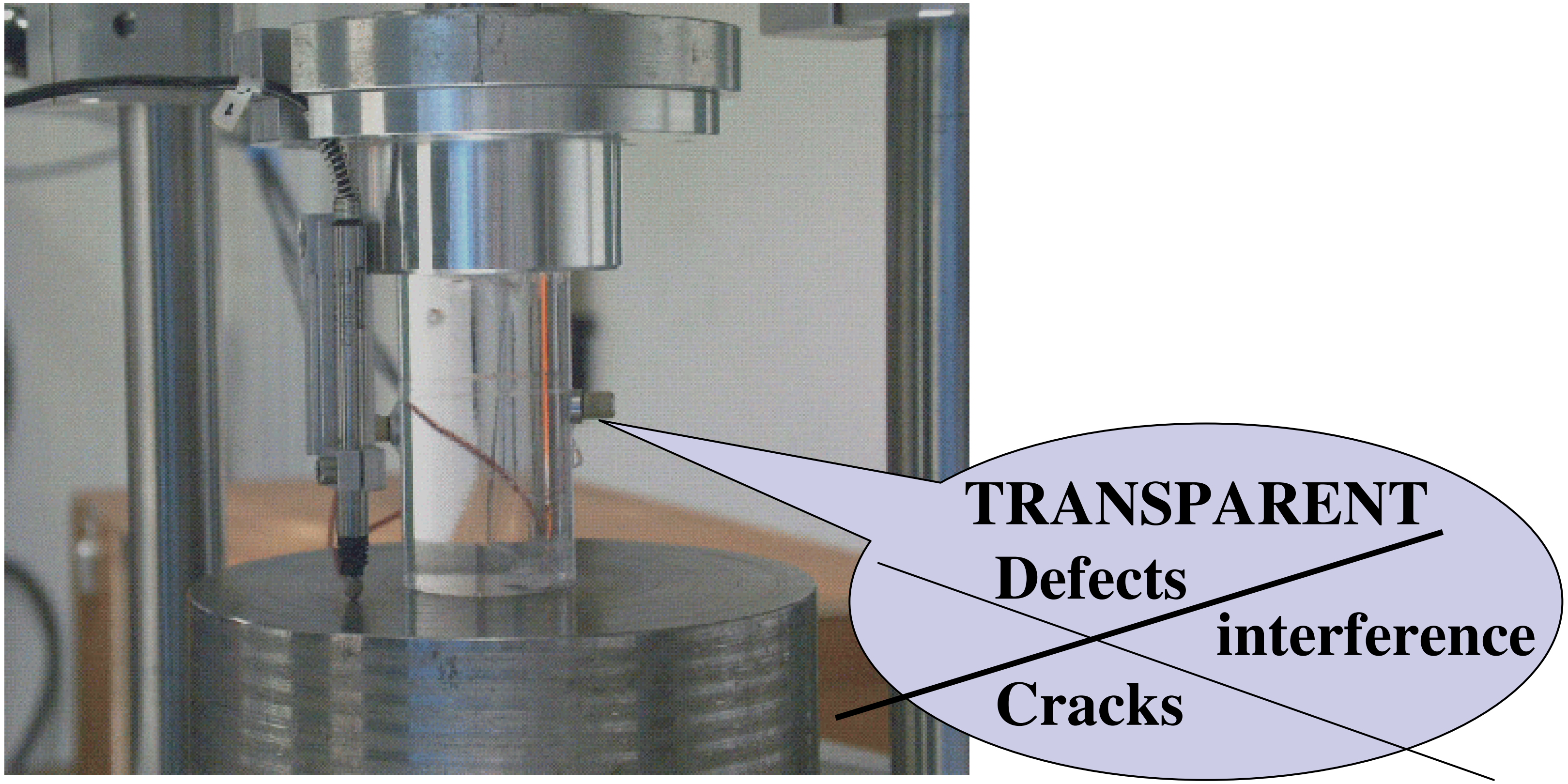
Continuum plasticity: Plastic deformation resembles a smooth flow process, quasi-laminar flow of dislocations

Under the action of constant stress:



Same behavior observed in several materials!

Plastic flow of ice single crystals



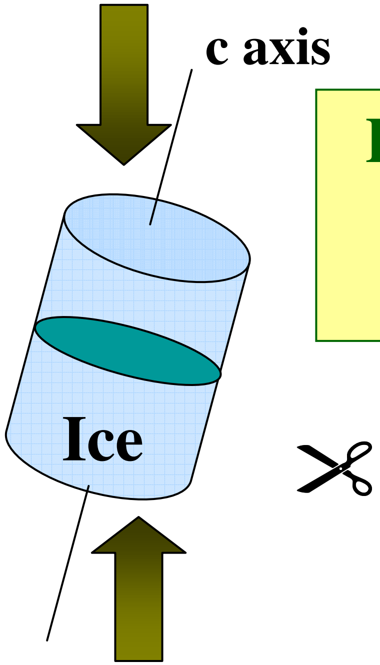
Compression creep test on an ice single crystal.
Piezoelectric transducers are fixed directly on the sample

Nature **410**, 667 (2001)

ACOUSTIC EMISSION (AE) FROM COLLECTIVE DISLOCATION MOTION

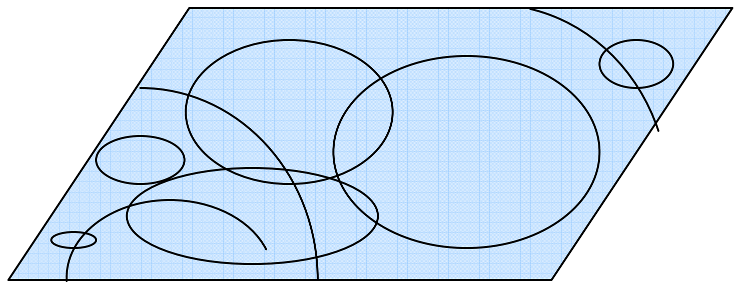
CREEP COMPRESSION

Small shear stress on the basal planes

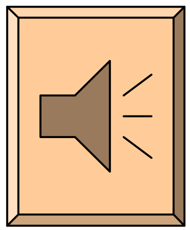


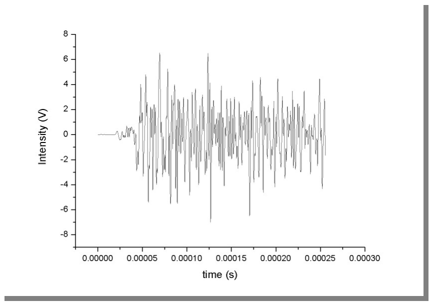
SINGLE SLIP

Deforms by slip of dislocations on the basal planes along a preferred direction



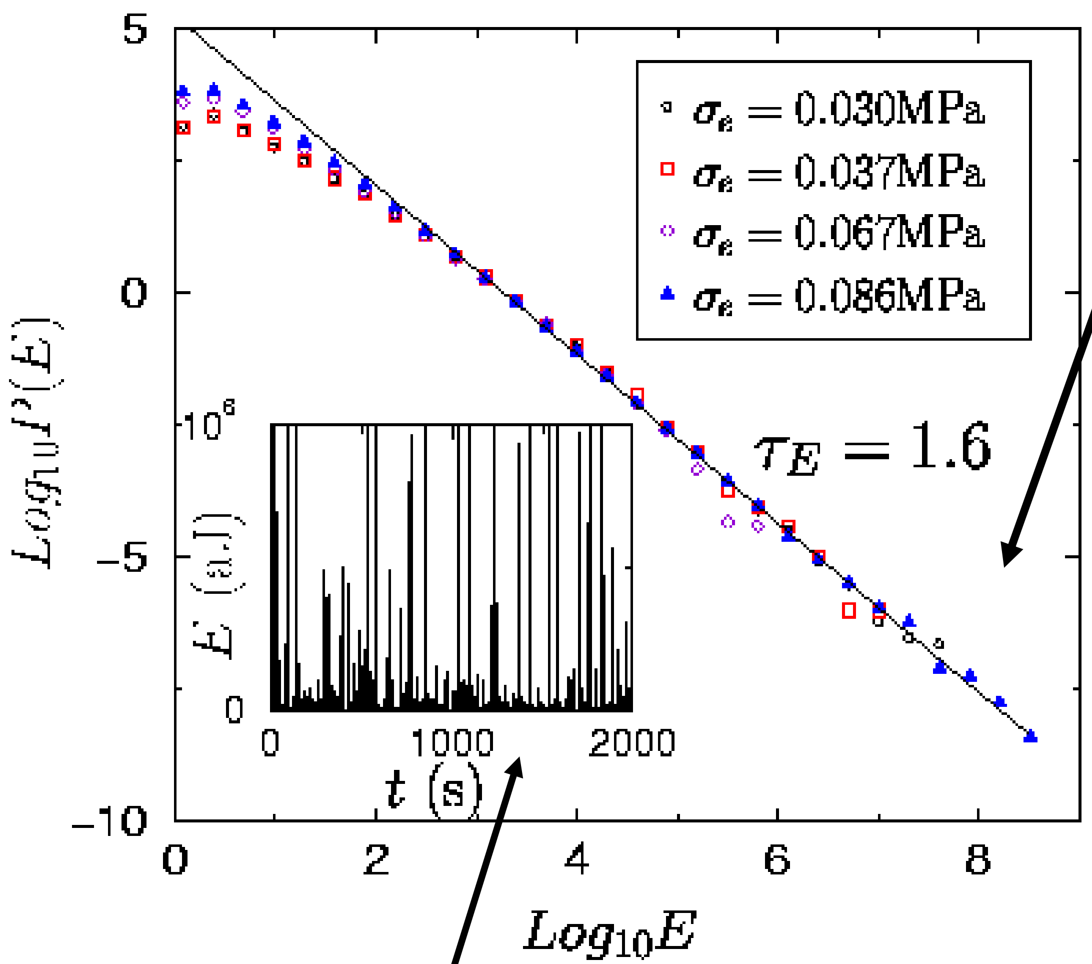
SUDDEN CHANGES OF INELASTIC STRAIN





ACOUSTIC EMISSION

Energy distribution of acoustic events   P(E)



Power law distribution

$$\mathbf{P(E) = E^{-\tau_E}}$$

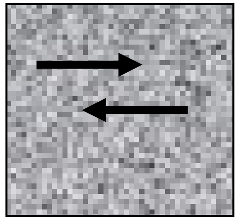
$$\tau_E = 1.6 \pm 0.05$$

Applied Stress
0.58 MPa -1.64MPa
Resolved shear stress
0.03 MPa - 0.086 MPa

Bursts of activity: Collective dislocation rearrangements

Avalanches

Dislocation dynamics model



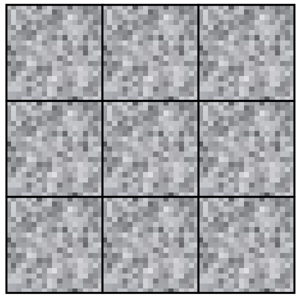
- 2D cross section & point-like edge dislocations.
- Random initial configuration ($\rho_0 = N/L^2b^2 \sim 1 – 5$ %)
- Burgers vectors +b or –b with equal probability (single slip).

➢ Relaxation=Numerically solve (adaptive-step-size fifth order Runge-Kutta) the coupled over-damped equations of motion:

$$\dot{x}_n = \mu b_n \sum_{m \neq n} \sigma(\vec{r}_{nm})$$

with long range interactions until the system reaches a still configuration (Ewald sums).

$$\sigma_{nm}(x,y) = b_m D \frac{x_{nm}(x_{nm}^2 - y_{nm}^2)}{(x_{nm}^2 + y_{nm}^2)^2} \propto \frac{1}{r_{nm}}$$



- Annihilation of dislocation pairs at short distances $r_{nm} \sim 2b$:
  Remaining dislocation density (ρ ~ 0.5 – 1 %)

- Apply constant external stress σ^e to relaxed configurations

$$\dot{x}_n = \mu b_n \left[\sum_{m \neq n} \sigma(\vec{r}_{nm}) + \sigma^e \right]$$

- Creation of new dislocation pairs: Frank-Read sources (FRS's).

IF HIGH STRESS σ > σ* — **Activation threshold value**

- Creep dynamics: Strain rate vs. time

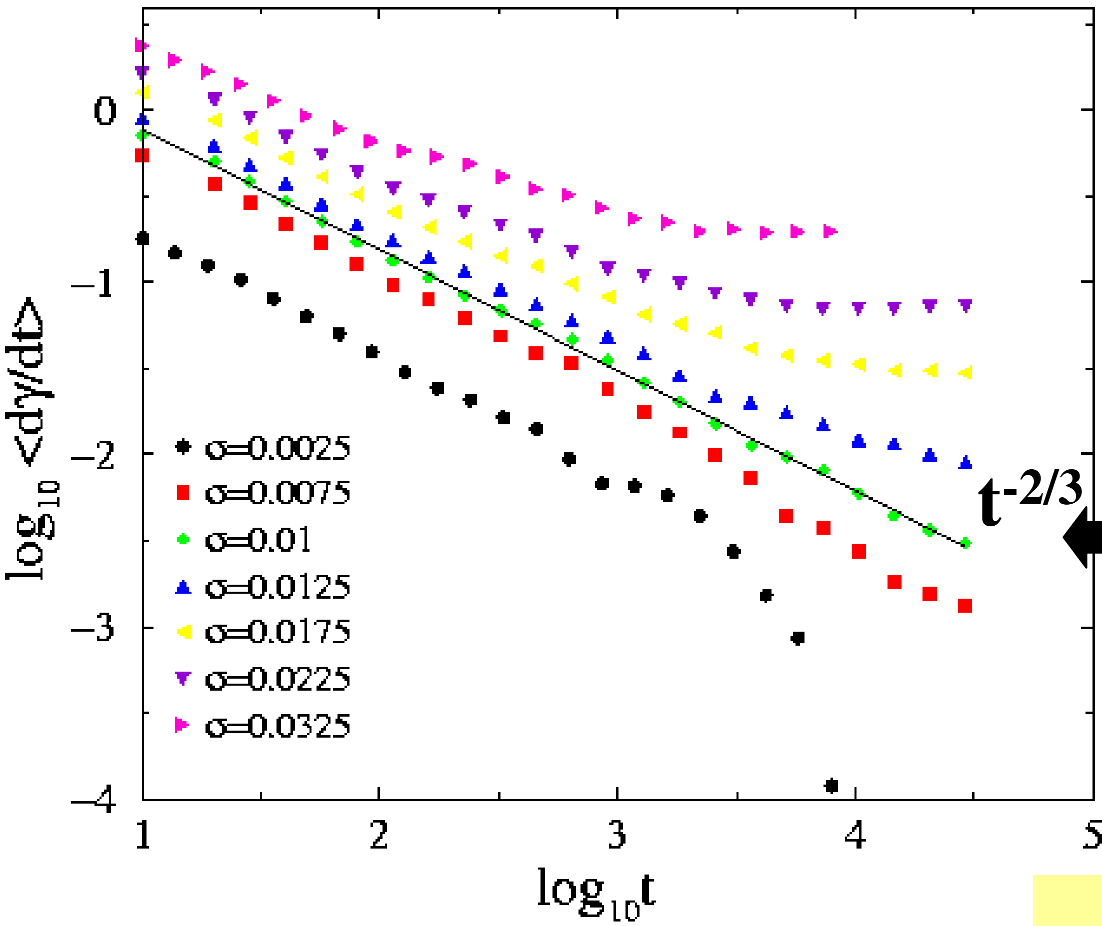
$$\dot{\gamma}(t) \propto \sum_n b_n v_n$$

Low stress dynamics

- Without creation of dislocations.

$$\gamma / \sigma = j_0 + \alpha t^{1/3} + \beta t$$

Andrade's & Linear Creep



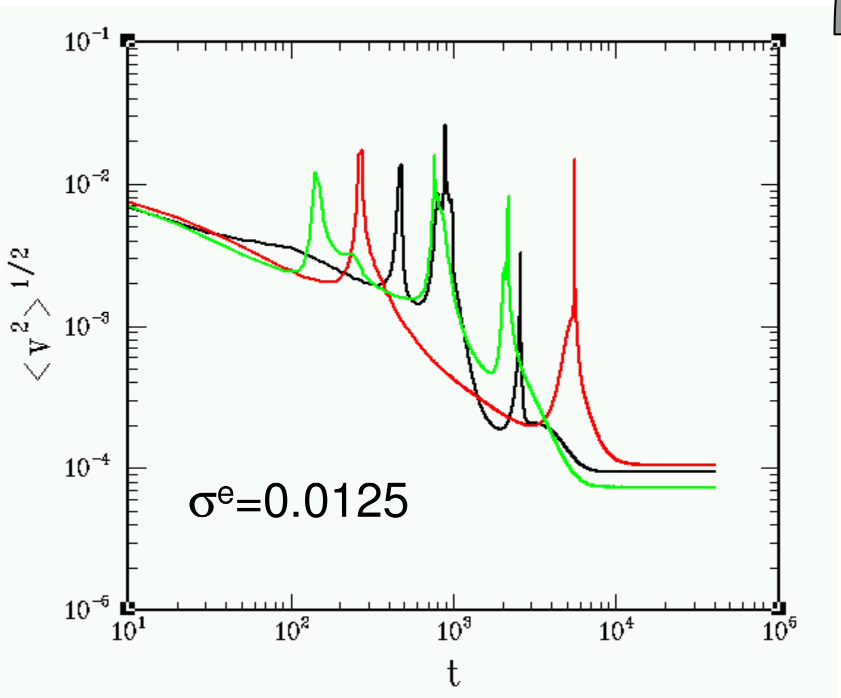
Slow *power law* relaxation of the "average" strain-rate for almost all the time span

Andrade's & Exponential decrease toward no strain-rate

BOX SIZE 100b x 100b

Three individual runs: Microscopic behavior

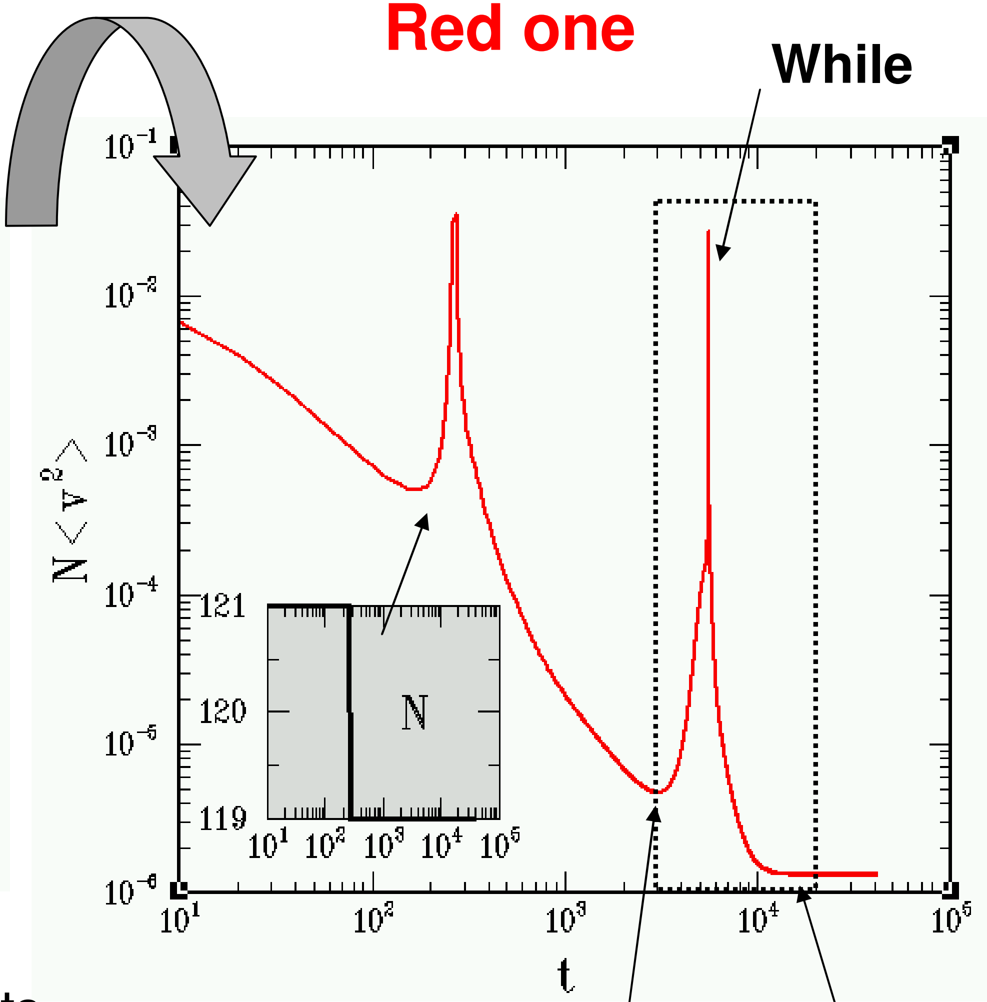
"Intermittent" signals:
Bursts of activity



$N\langle v^2 \rangle$ ~ Kinetic energy at the points where we have dislocations

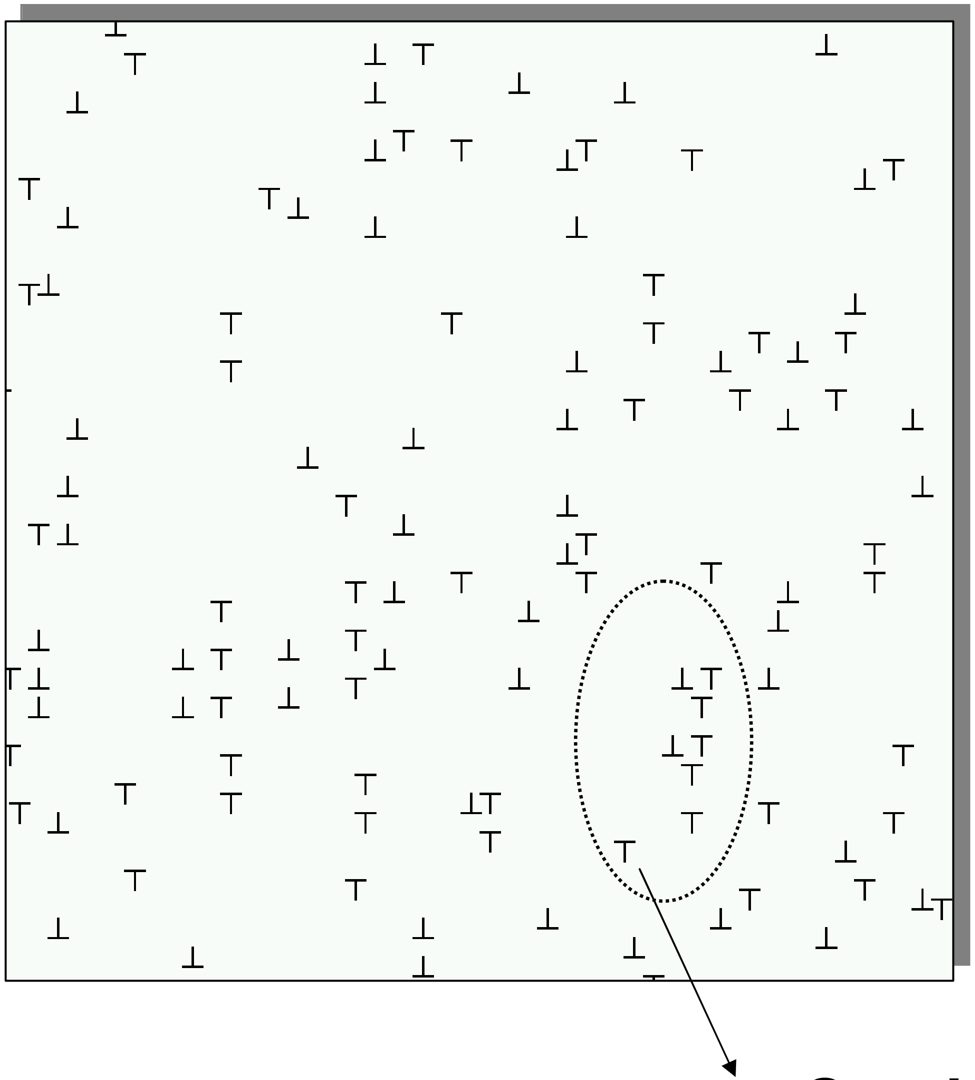
Red one

While



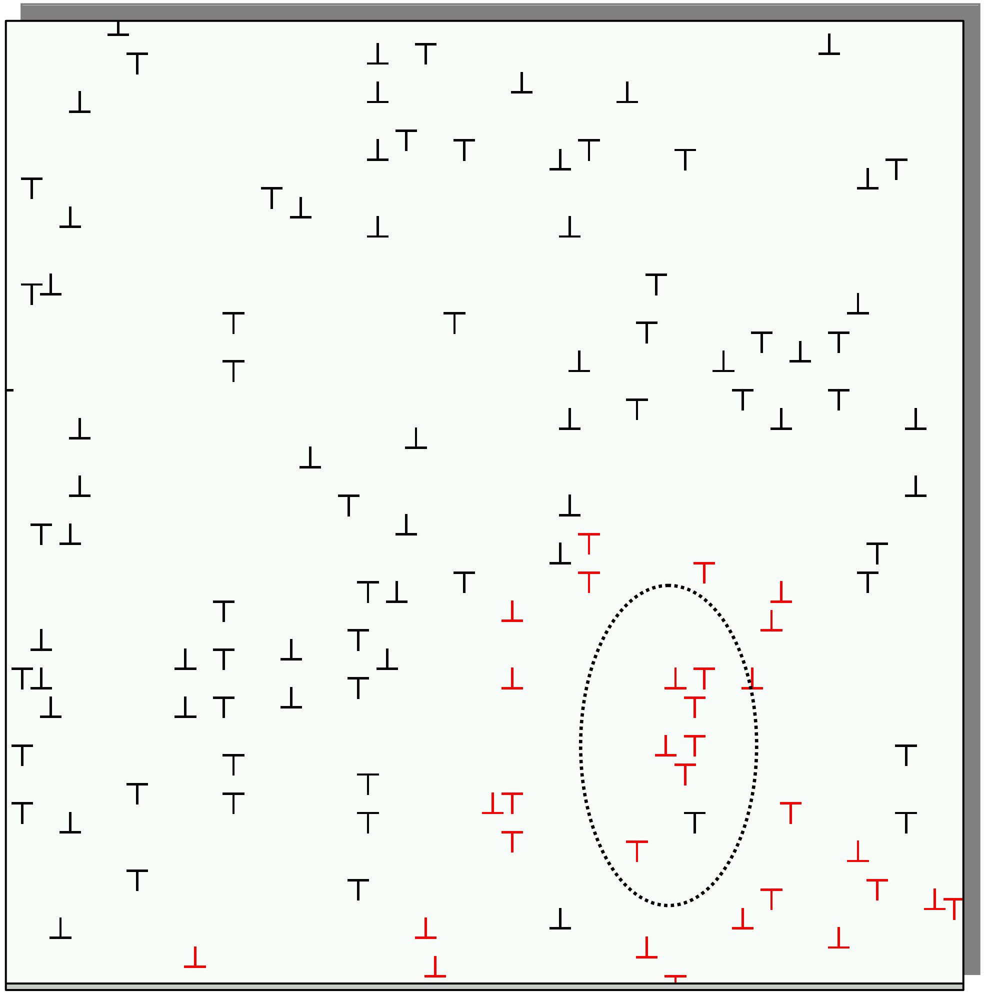
Before **After**

Before



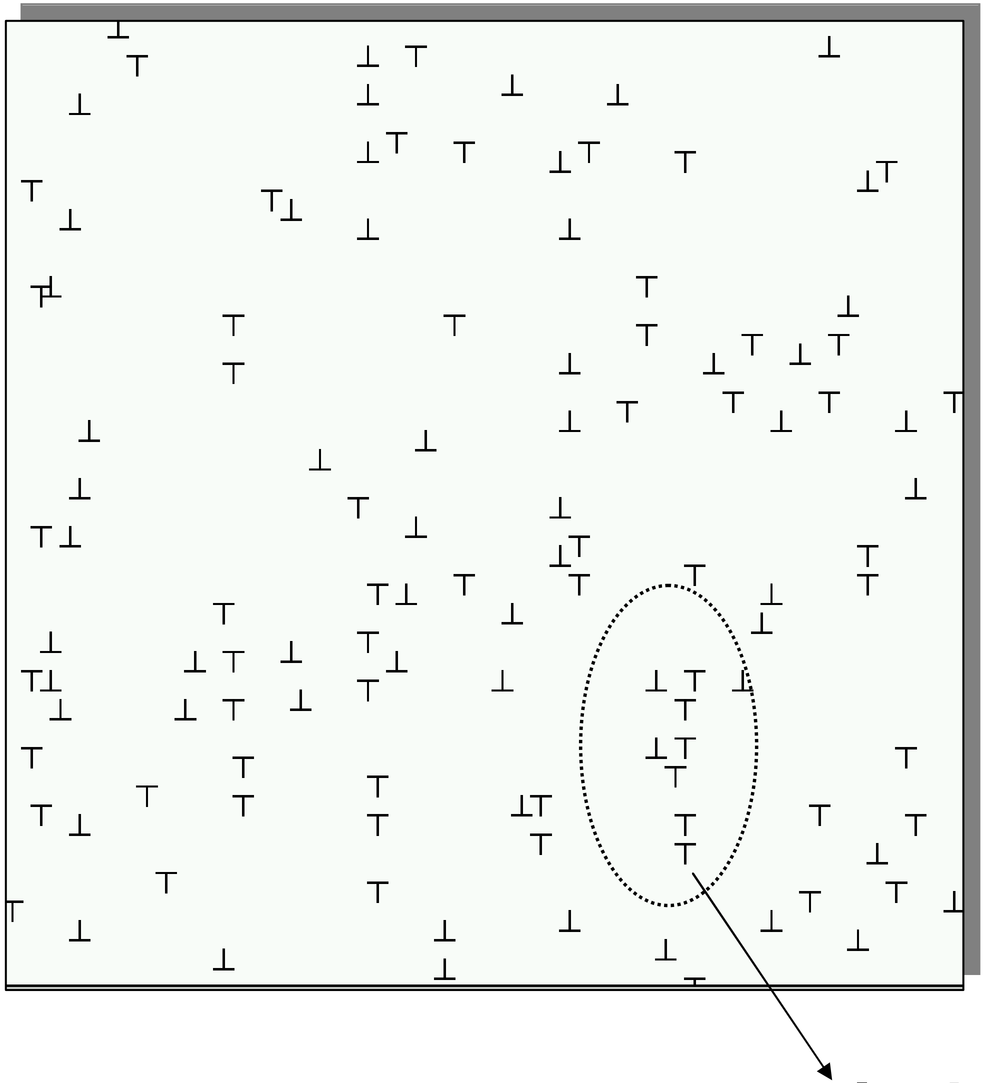
Outside the wall

While



Fast $(v > v_\sigma)$ **dislocations collaborating in the collective rearrangement**

After

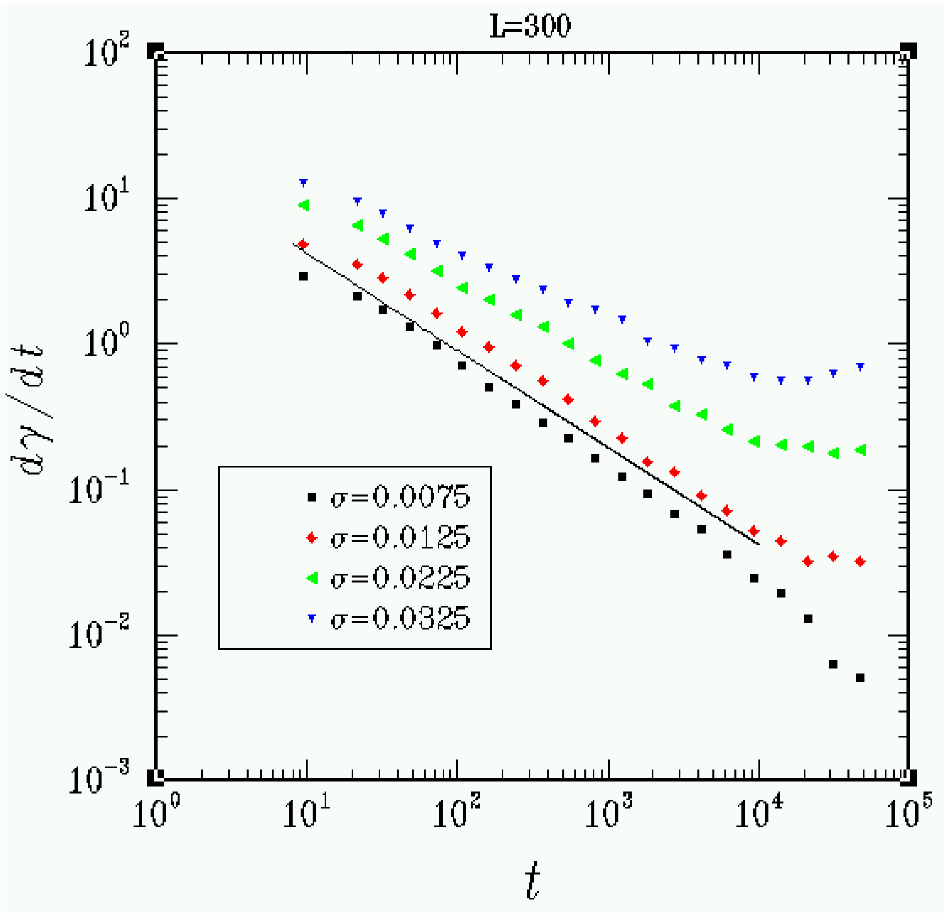


N has remained constant in this case!

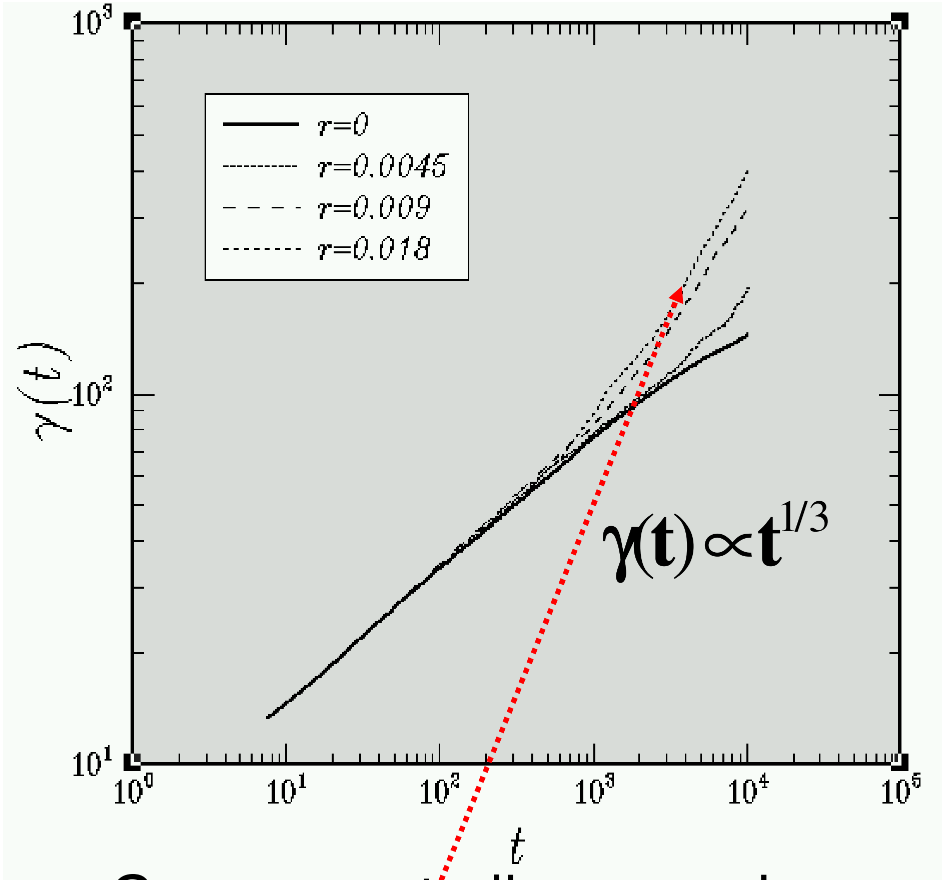
Inside the wall

Same results hold:

- With creation of new dislocations.
- For different system sizes & multiplication rates r.



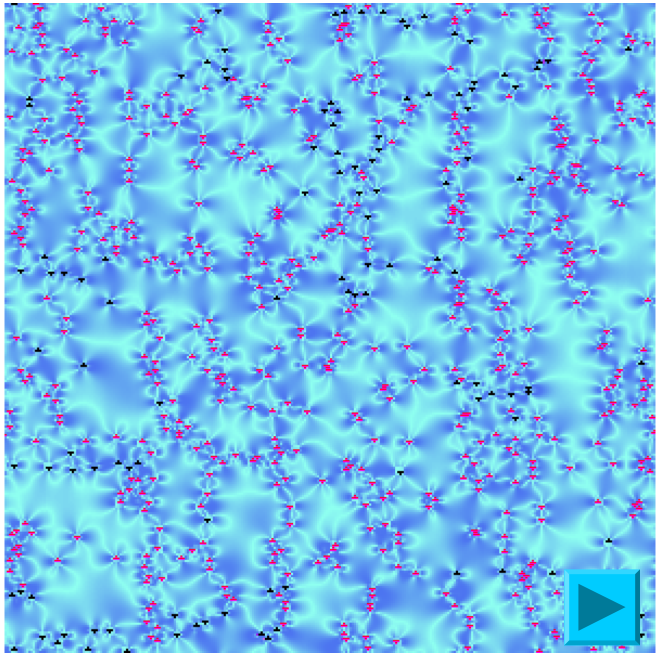
BOX SIZE 300b x 300b



Crossover to linear regime

(crossover time gets shorter with r)

In the stationary state



- Rearrangements of dislocation structures (Dipoles, walls, cells, etc.)
- Annihilation of dislocation pairs.
- Creation of new dislocations in FRS's.

⬇

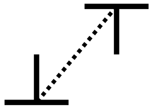
SINGULAR RESPONSE "AVALANCHES"

- ❖ Power law distributions for intermediate size avalanches ⇒ Absence of characteristic size.
- ❖ Exponential cutoffs for large size avalanches: Cutoff ⇓ when σ ⇑.

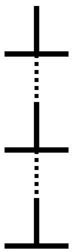
Nature **410**, 667 (2001)

Snapshots of the dynamics:

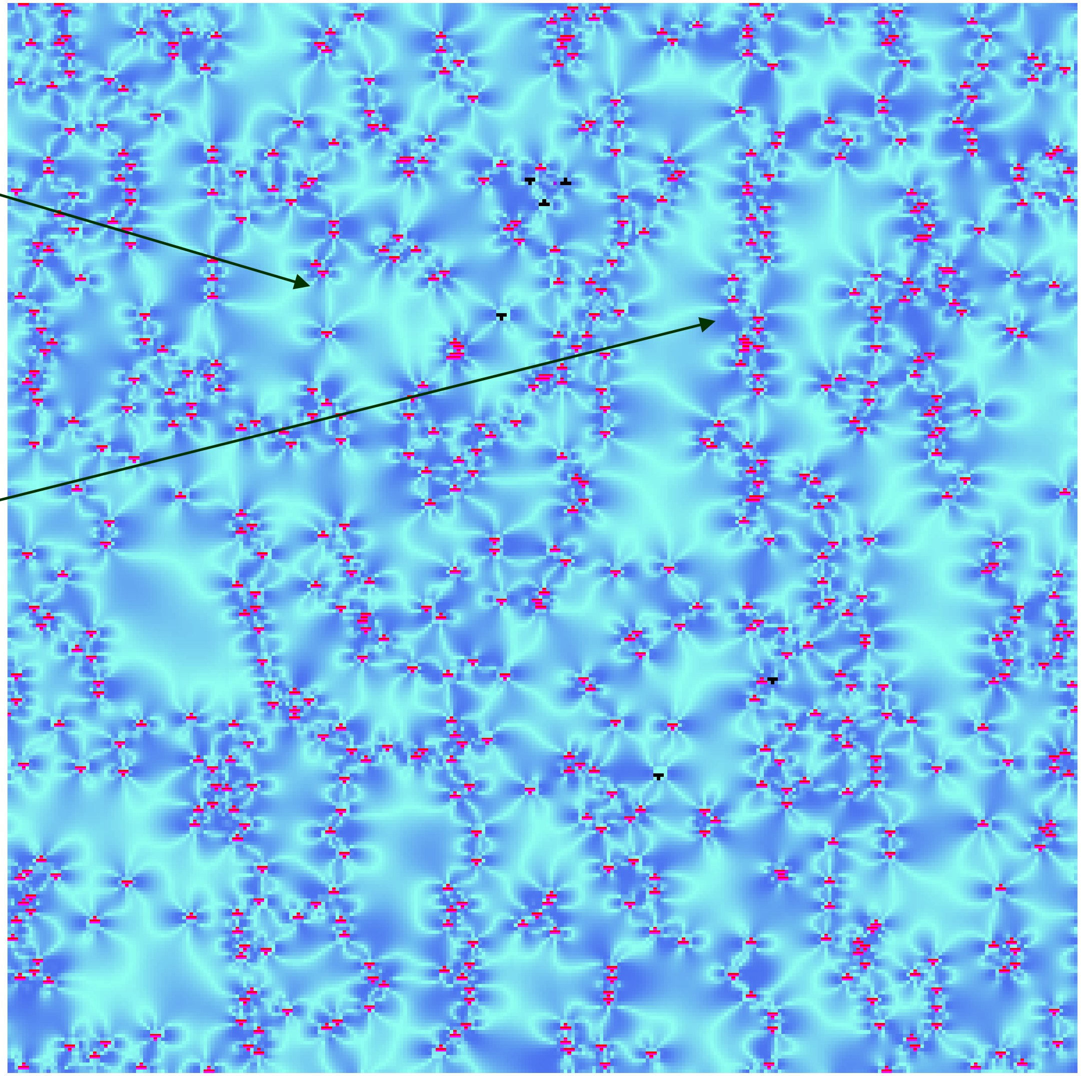
Dislocation dipoles



Dislocation walls...



Sources of self-induced jamming!

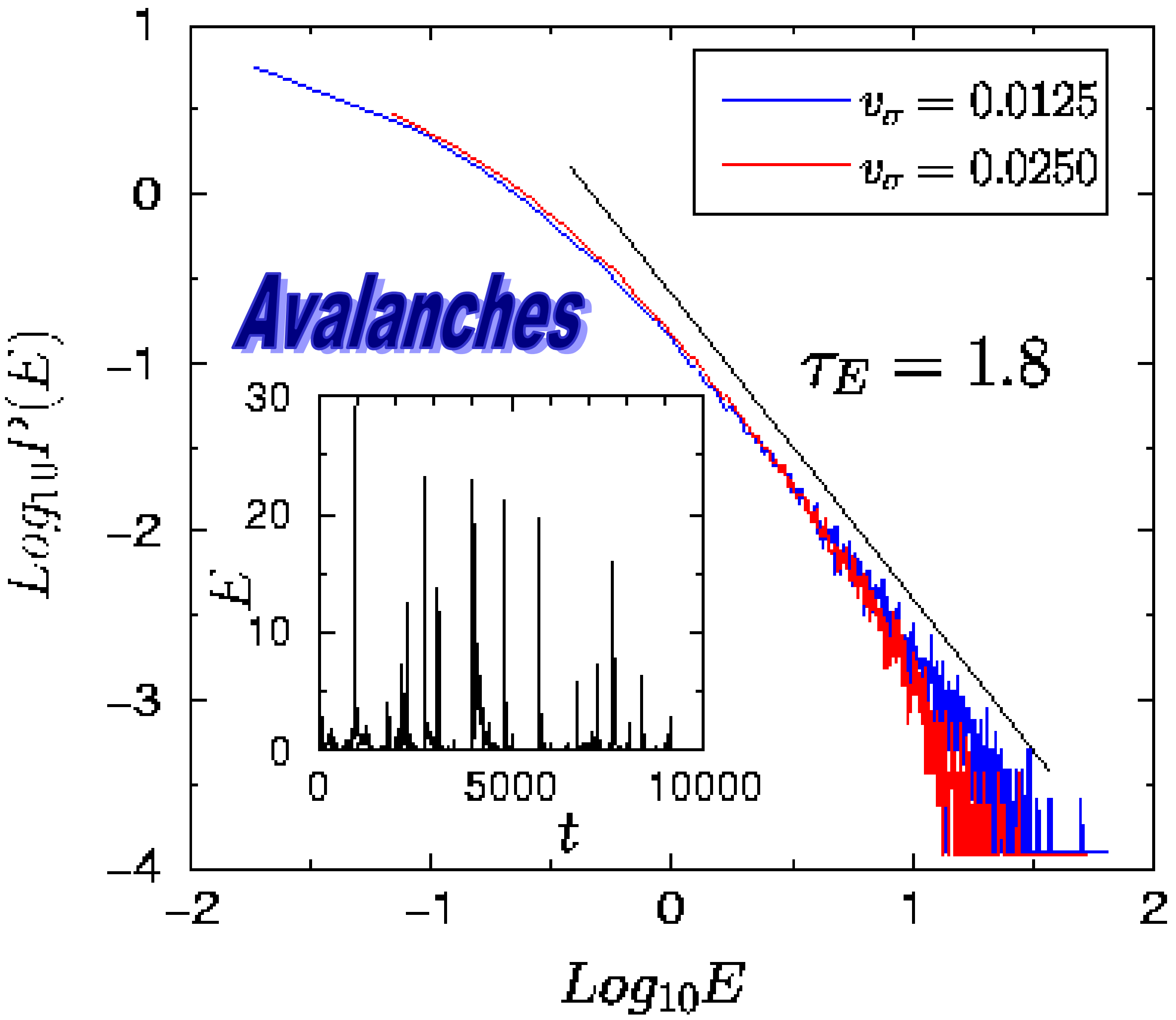


Stress Shear

low

high

SLOW FAST Dislocations



Mean Velocity vs. time

$$V(t) = \sum_{n}^{N_m(t)} |v_n|$$

"Acoustic" Energy

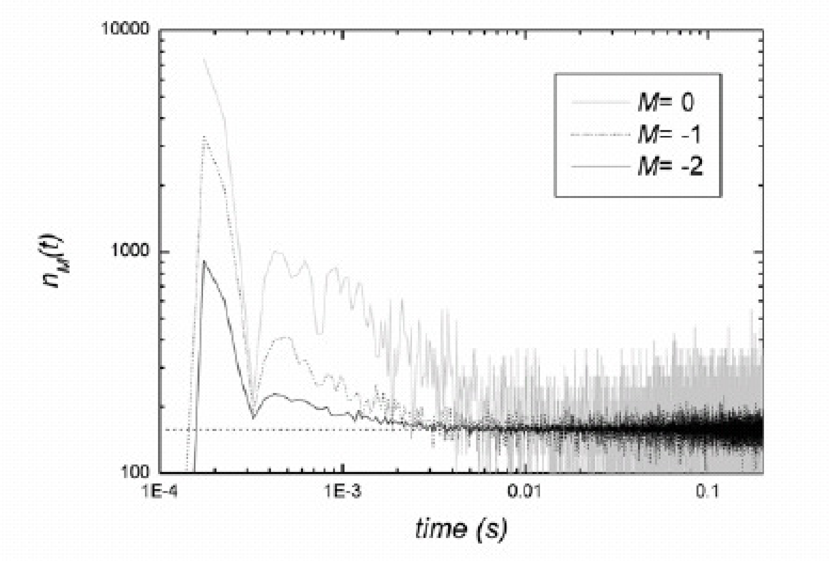
$$E = V^2$$

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

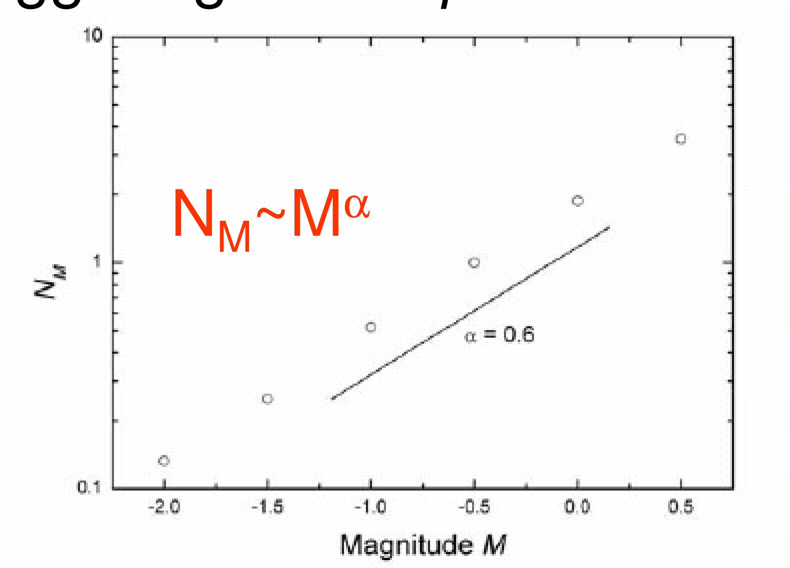
$$\tau_E = 1.8 \pm 0.2$$

In good agreement with Acoustic Emission experiments!

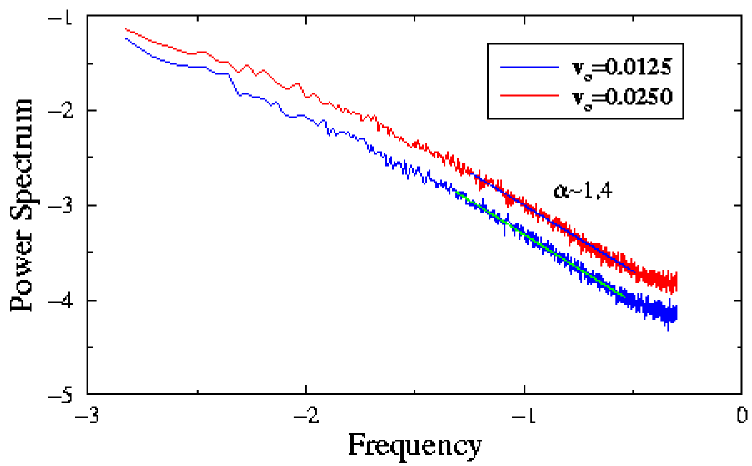
Correlations: Aftershock triggering in *ice-quakes*



Average AE event rate after avalanches of magnitude M=log A, per mainshock and per unit of time.



Average number of aftershocks triggered by dislocation avalanches of magnitude M=log A.



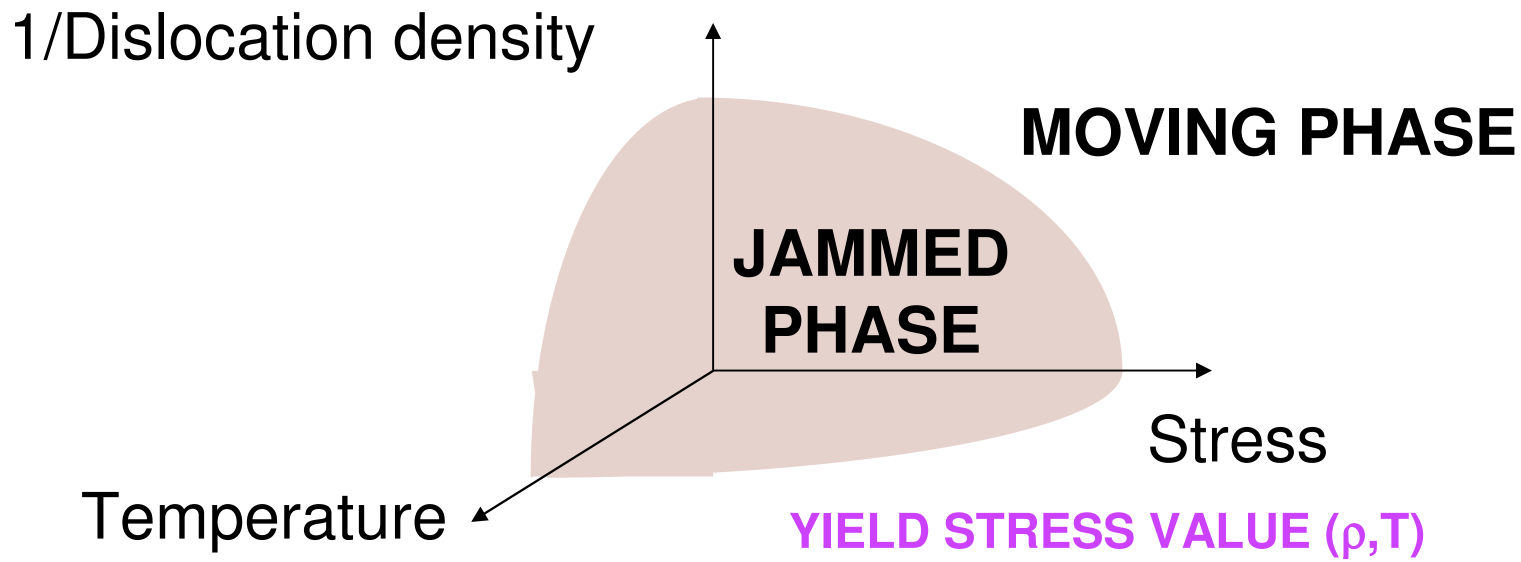
Time correlations of the AE signal in the model

- **Power law ⇒ Absence of characteristic correlation time**
- **Non-diffusive behavior**

The *jamming* scenario

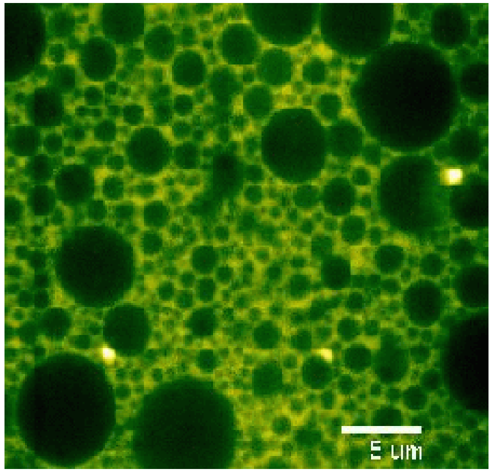
INTERMITTENCY, SLOW RELAXATION, SCALING $\Rightarrow$
PROXIMITY OF NON-EQUILIBRIUM CRITICAL POINTS

NON EQUILIBRIUM JAMMING TRANSITION



New framework to study a wide variety of **AMORPHOUS** soft glassy materials: emulsions, colloidal suspensions, foams, gels, etc.; and granular media.

Liu & Nagel, Nature **396**, 21 (2001)



COMMON FEATURES

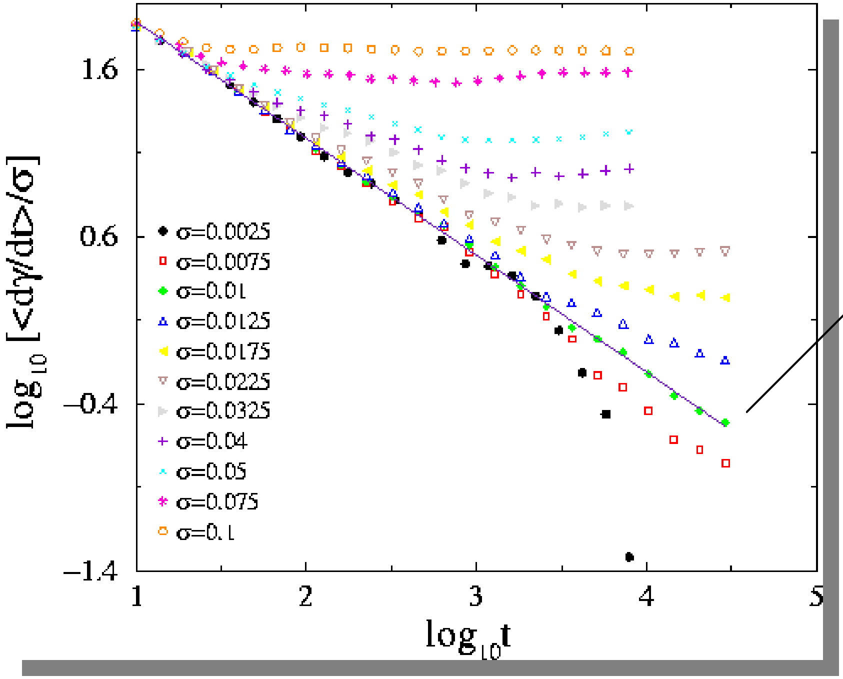
- Slow dynamics governed by kinematical constraints (density, geometry, etc.)
- Jamming ⇒ Suppression of temporal relaxation or the ability to explore the configurations space.
- Shear yielding ⇒ Liquid-like flow above the yield stress value.
- Creep compliance curves $J(t) = \gamma / \sigma = j_0 + Ct^{1/3} + t/\eta$

  Andrade and viscous flow
- Non-linear rheology:
  - Stress-strain relationships $\sigma \approx a\dot{\gamma}^n$
  - Viscosity $\eta = \sigma / \dot{\gamma} \approx \dot{\gamma}^{-\alpha}, 0.5 \leq \alpha \leq 1$

Dislocation jamming in crystals

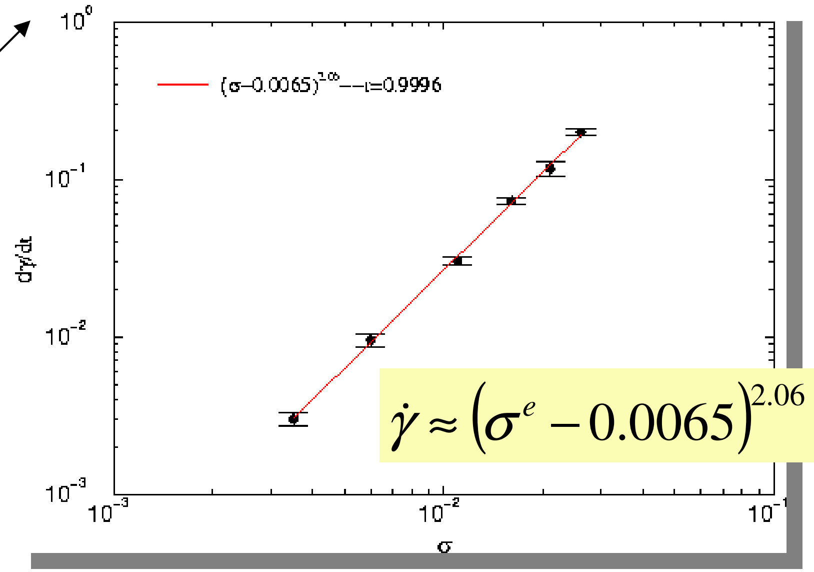
We also find

- Broad region of slow dynamics due to kinematical constraints: Metastable patterns ⇒ Andrade's creep.
- Dislocation jamming below the yield stress threshold.
- Shear yielding above threshold: Primary, secondary regimes.



Phys. Rev. Lett. **89**, 165501 (2002).

Yield threshold value ?



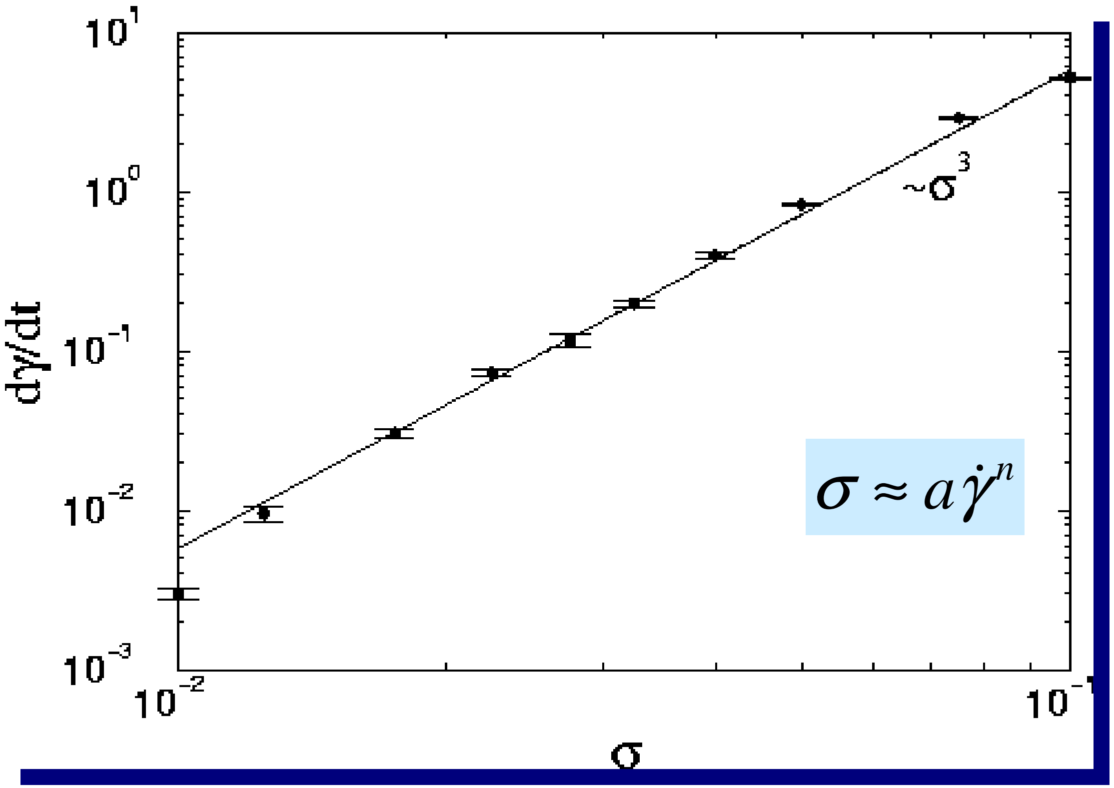
$$\dot{\gamma} \approx \left(\sigma^{e} - 0.0065\right)^{2.06}$$

Exhaustive study of finite-size effects

Dislocation jamming in crystals

We also find

- Non-linear stress-strain relationships in the stationary state.



$$\sigma \approx a\dot{\gamma}^{n}$$

$$\sigma \approx a\dot{\gamma}^{1/3}$$

$$\eta = \sigma / \dot{\gamma} \approx \dot{\gamma}^{-2/3}$$

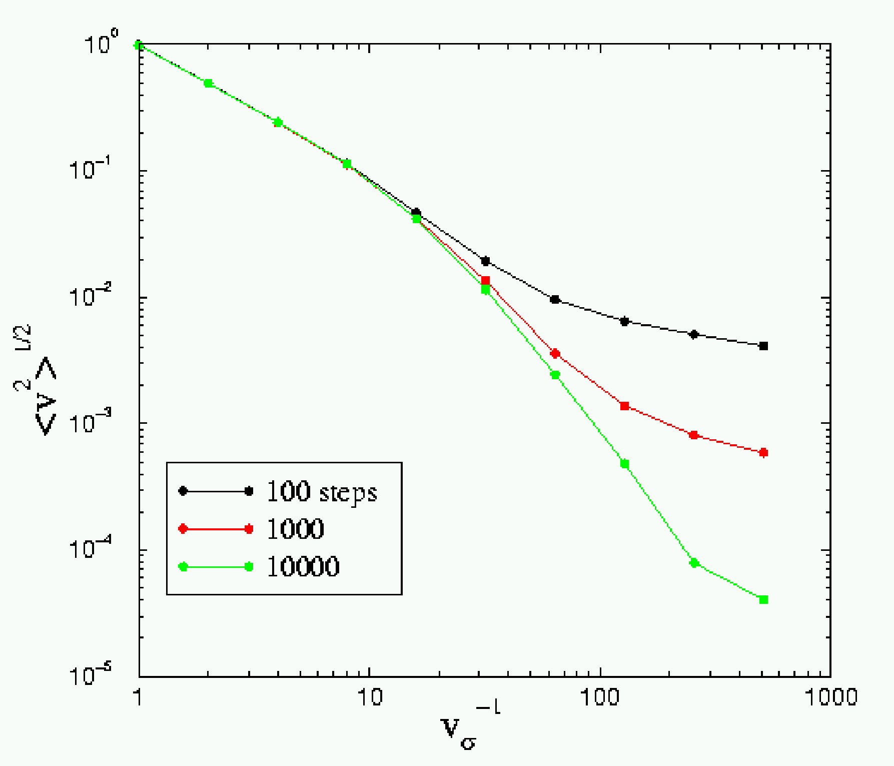
Cox- Merz rule

$$\eta = \sigma / \dot{\gamma} \approx t^{2/3}$$

Best fit in the steady state for the intermediate stress values

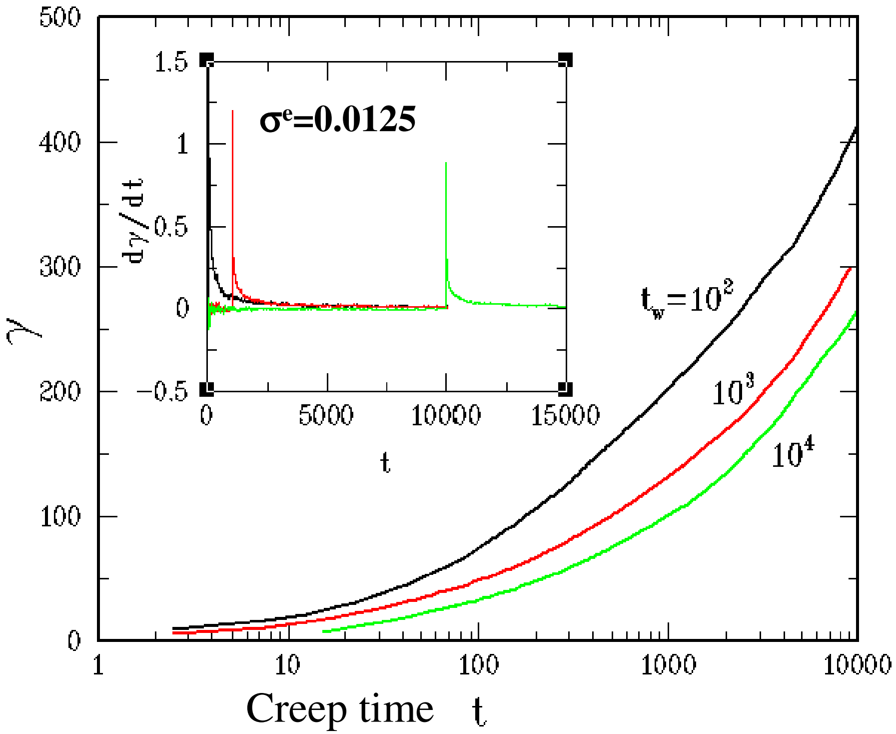
Aging phenomena

✓Loading rate dependence



For the lower values of stress, the final state depends on the stress rate of change

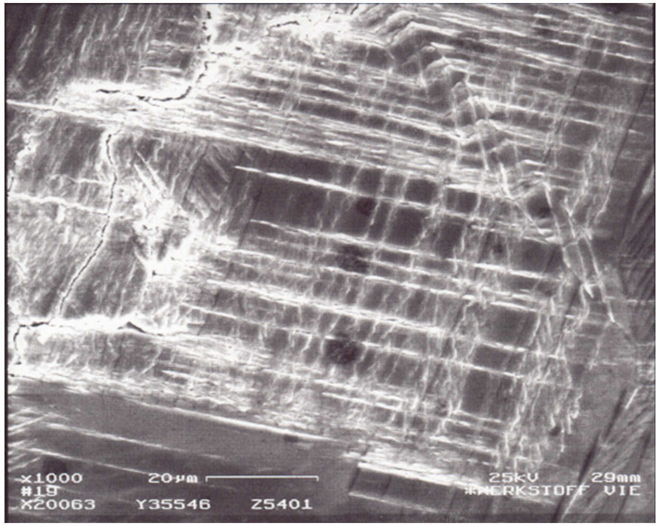
✓Aging-like behavior



t_w Waiting time (without loading) after a sudden ***quench*** of random configurations

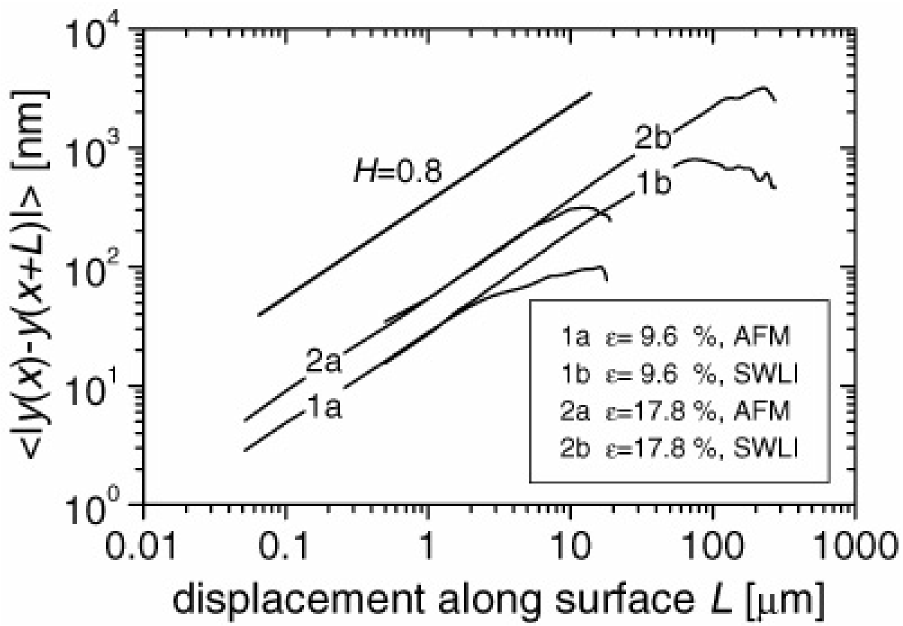
(Reminds Struik´s aging experiment on a PVC sample (78))

Slip heterogeneity and surface morphology



The heterogeneous distribution of slip has also implications on the surface morphology of plastically deformed crystals.

Slip steps on the surface of deformed Cu manifest the collective motion of dislocations



Self-affine roughness over several orders of magnitude in scale

Hurst exponent calculated from surface profiles along the deformation direction

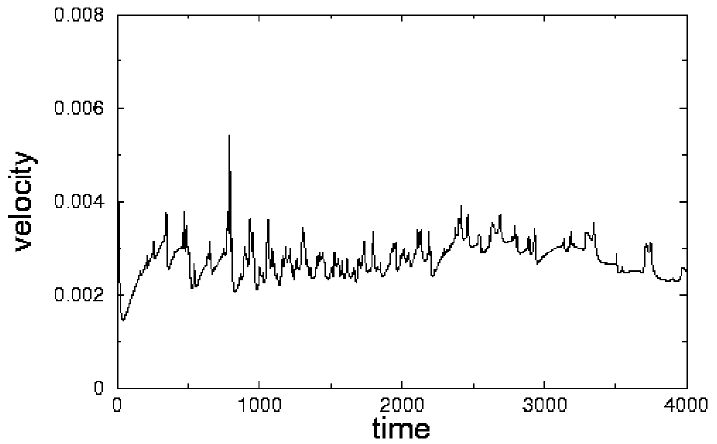
Zaiser et al., PRL **93**, 195507 (2005)

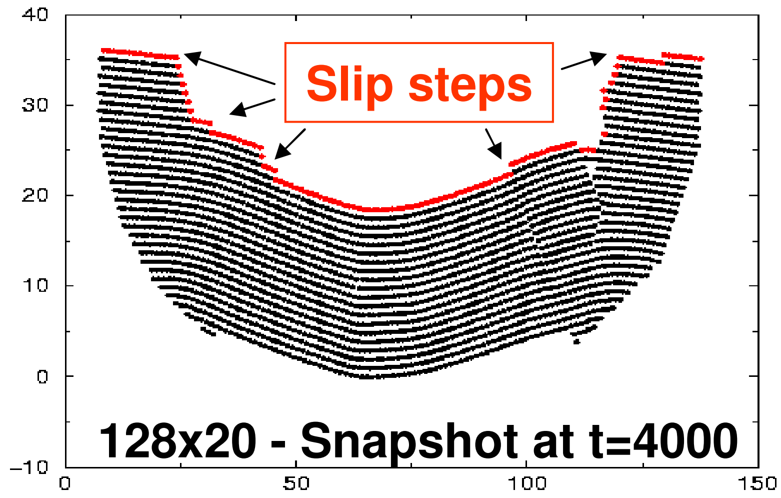
On microscopic scales …

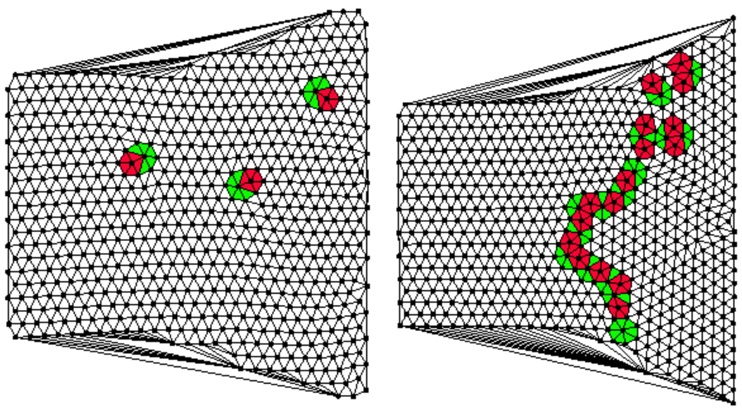
Work in progress: 2D colloidal crystals under different modes of deformation

We also find:

Intermittent slip







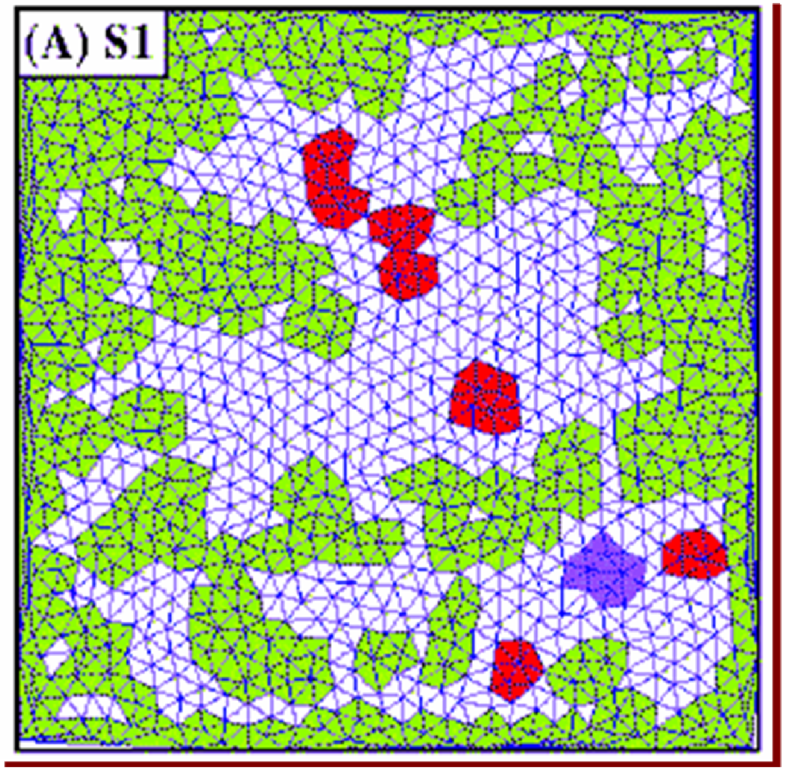
Different microscopic mechanisms mediating plastic deformation, depending on boundary conditions, and/or deformation mode:

- Dislocation sequential motion
- Grain boundary formation and gliding
- Re-crystallization

Vortex lattices in superconductors

Mixed state of type II superconductors ⇒Magnetic field enters in the form of a flexible array of flux lines that, much like ordinary matter, can form crystalline, liquid, and glassy phases.

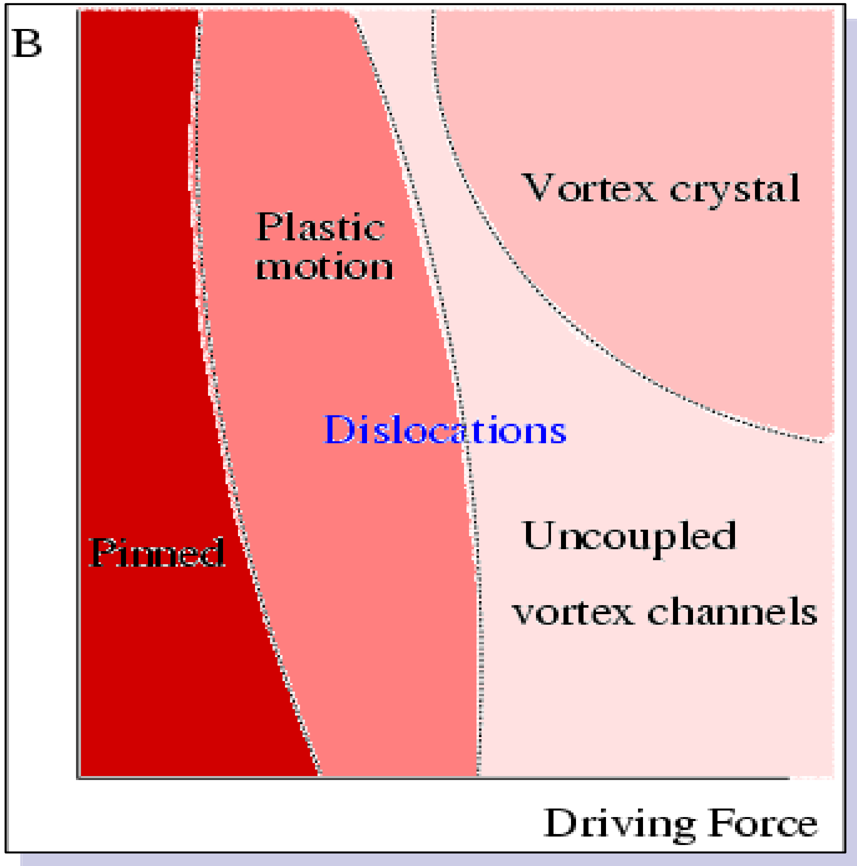
- Magnetic decoration: Powerful tecnique to investigate the topology of the lattice.
- Topological defects: Isolated dislocations, dislocation dipoles, and grain boundaries as in conventional crystals.



Delaunay triangulations of the magnetic flux line positions.

Vortex phases & quenched disorder

- Experimentally accessible to study dynamic phase behavior and/or phase transitions.
- Elastic properties easily tunable with magnetic field
- Dynamic phases: pinned, crystalline, plastic ⇒ intermediate regime where the lattice is found to be quite disordered.



PLASTIC DEPINNING & PLASTIC FLOW

•Nucleation & motion of dislocations.

•Yields a non linear response (I-V curves).

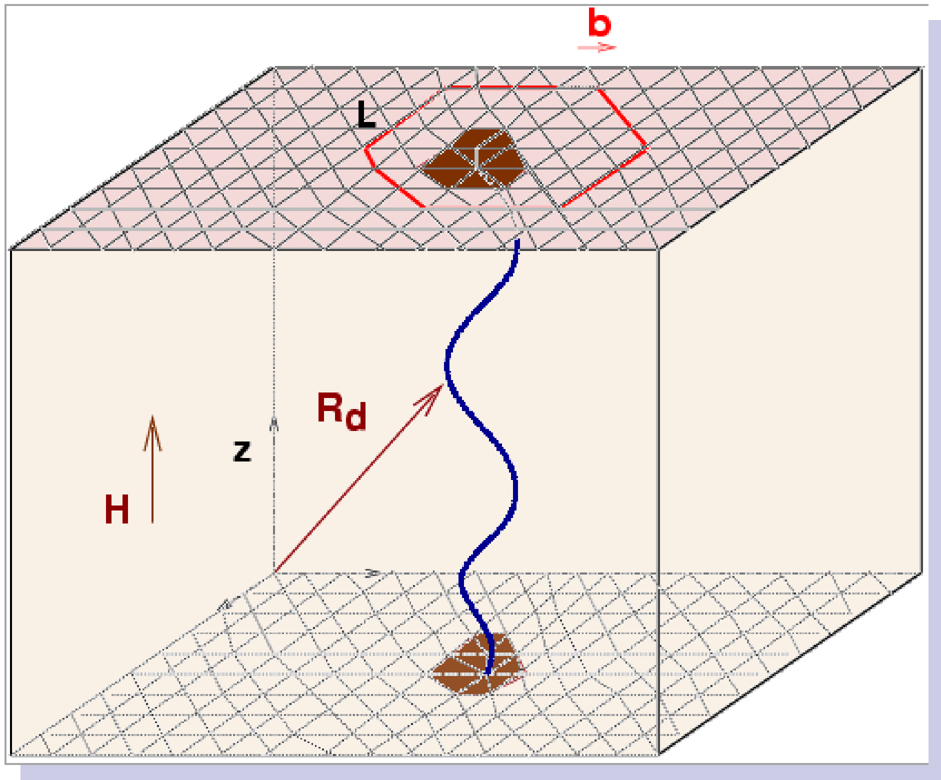
Dislocations in the vortex array

Thin superconducting samples: Threading edge dislocations

$$\oint_L du = b$$

Burgers vector b ⊥ dislocation axis

u elastic displacement field
in the vortex lattice



- ☒ 7:5 coordination
- ☒ Peach-Koehler force,

$\tau\times(\sigma\cdot b)$, due to the elastic shear stress field, $\sigma \sim \nabla u$, that is usually generated by quenched disorder, other defects, external current distributions, etc.

Vortex polycrystals

Experimental evidence

- Magnetic decoration images, e.g. after field cooling thin samples $NbSe_2$ at 36 Oe, and applying a current $J<J_c$.

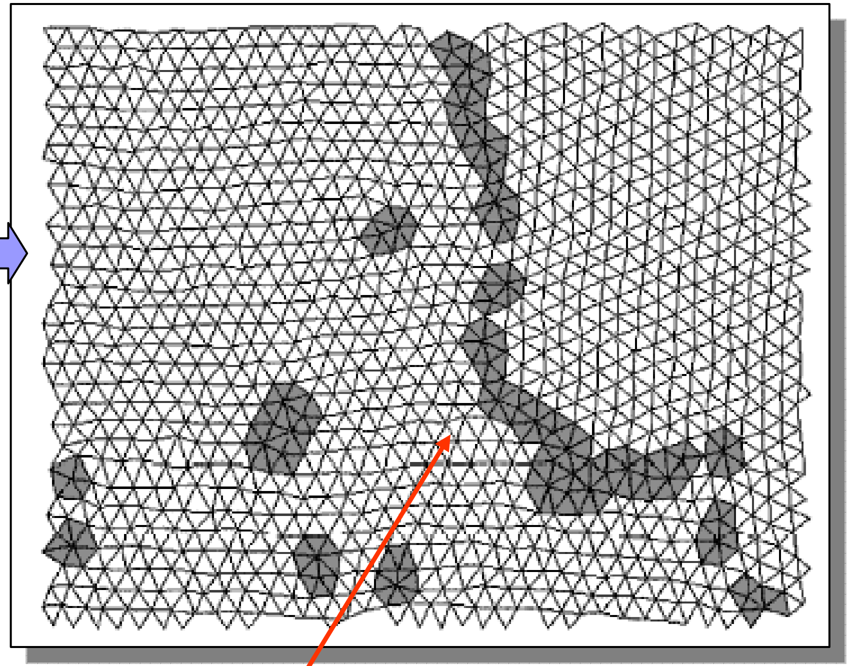
  F. Pardo et al. PRL 78, 4633 (1997).

- Similar experiments (FC, ZFC, FCR):

  Y. Fasano et al. PRB 66, 020512 (2002)

  M. Menghini et al. PRL 90, 147001 (2003)

- Possible relevance in the "peak effect" – Enhanced pinning strength.



Grain boundary separating crystalline <u>columnar grains</u>

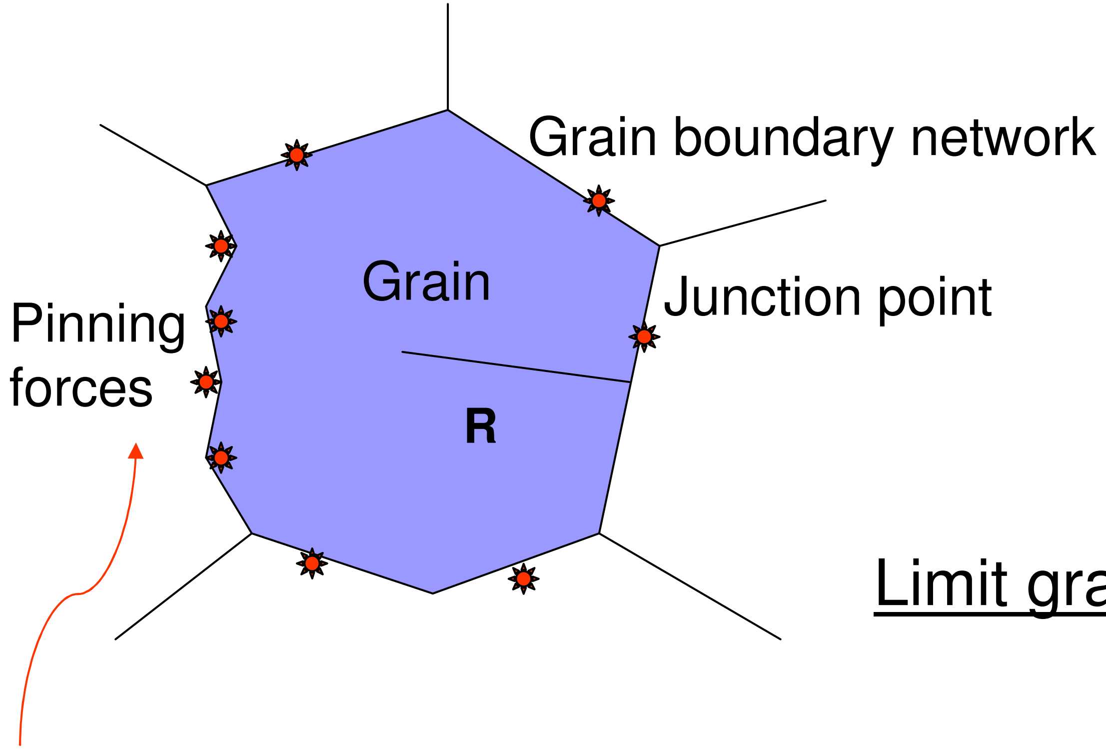
Grain growth

- Glide motion of grain boundaries (GB).
- Driving forces:
  - Externally induced through current flow in the superconductor.
  - Internally generated by the gradual ordering process (residual stress) after a rapid quench.
- Tends to minimize the energy cost of GB, $\frac{E}{V} \propto \frac{\Gamma_0}{R}$
  - Average grain size R
  - Straight grain boundaries
  - Γ_0 energy per unit area ~ Kb^2/D

Increasing the grain size dR→ Energy gain $\frac{dE}{V} \propto \frac{\Gamma_0}{R^2} dR$

Grain growth & Disorder (oxygen vacancies, impurities)

Energy gain (dR) ~ Work against the pinning forces on GB



Dissipative work per unit volume to move all GB a small dR,

$$E_p \approx \frac{\sigma_c b}{DR} dR$$

Limit grain size

$$R_g \approx \frac{D\Gamma_0}{b\sigma_c}$$

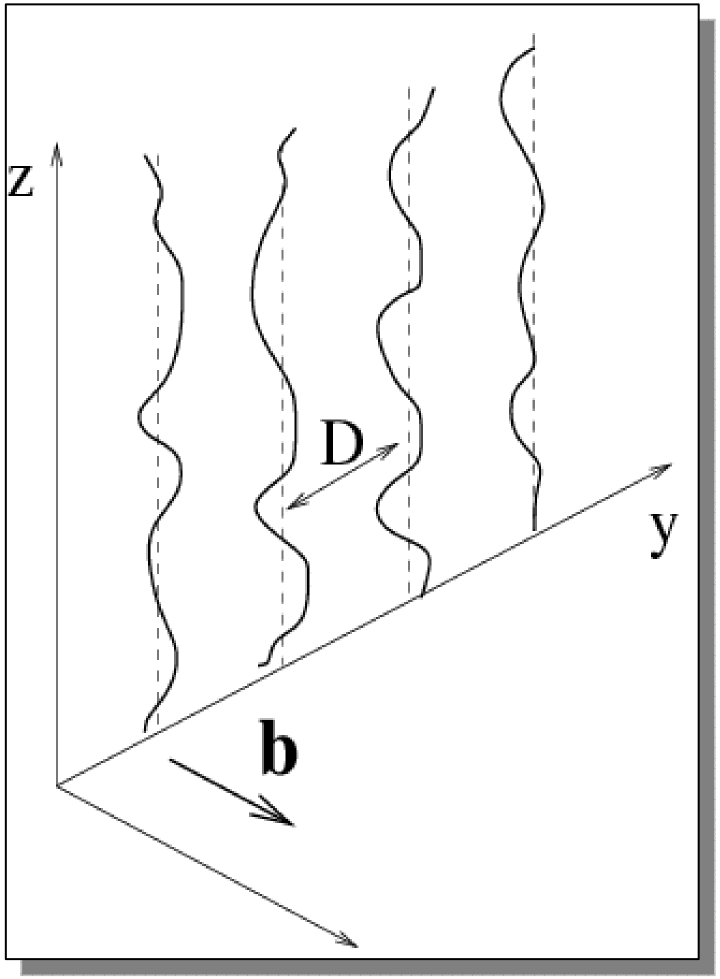
- Quenched disorder induces elastic deformations of GB's.
- σ_c--Competition between non-local elasticity, disorder and driving forces in the framework of pinning theories.

PRL **92**, 257004 (2004)

Elastic properties of an ideal GB

- An infinite & regularly spaced low-angle grain boundary of edge dislocations piled-up along the y axis and with Burgers vectors in the x direction.
- Dislocation wandering within the slip plane

$$R_i(z) = (X_i(z), iD)$$



- Elastic Hamiltonian of the vortex lattice, i.e.

$$H = 1/2\int d^3r\left[c_{66}(\nabla u)^2 + (c_{11} - c_{66})(\nabla \cdot u)^2 + c_{44}(\partial_z u)^2\right]$$

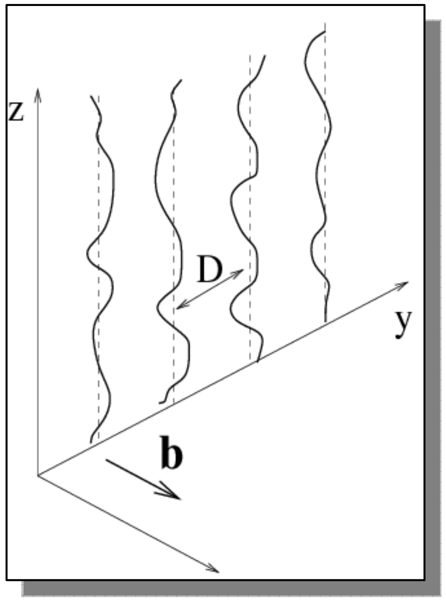
Elastic properties of an ideal GB

In the harmonic approximation & taking into account appropriate constraints:

$$H = \frac{\pi b^2}{2D^2} \sum_{G_y} \int_{BZ} \frac{dQ_y}{2\pi} \int \frac{dk_z}{2\pi} \left[M(Q_y + G_y, k_z) X(Q_y, k_z) X(-Q_y, -k_z) \right]$$

The long-distance (q→0) behavior of the kernel:

$$M(k_y, k_z) \cong 2c_{66}|k_y| + \sqrt{c_{44}c_{66}}|k_z|$$

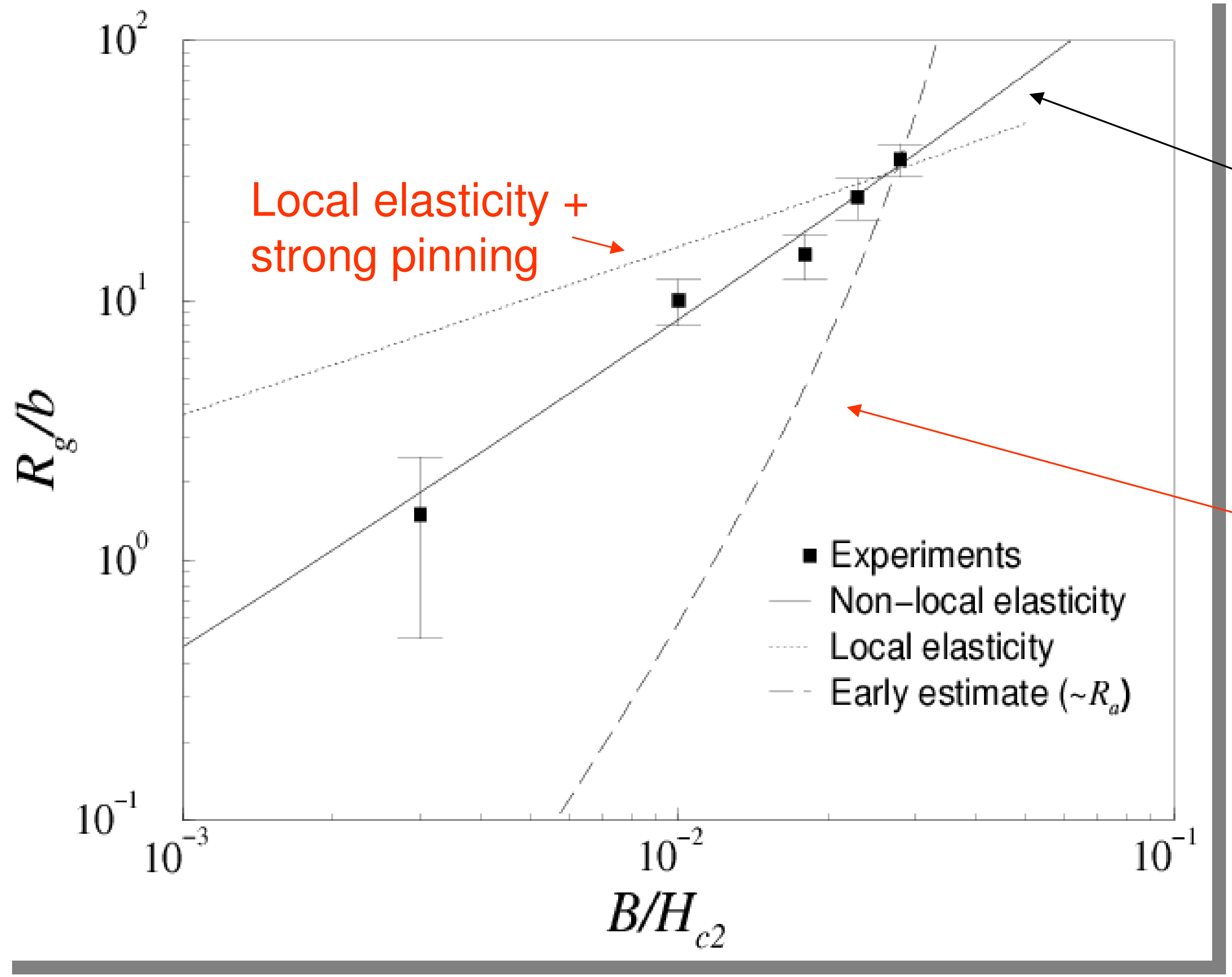


Or rescaling the y-axis by a factor $\frac{1}{2}\sqrt{\frac{c_{44}}{c_{66}}}$

$$M(k_y, k_z) \cong K|k|,$$ with $$K = \sqrt{c_{44}c_{66}}$$

A strongly non-local elastic kernel !

Experimental results for grain size in NbMo



Theoretical Estimates:

Strong pinning & Nonlocal elasticity

PRL **92**, 257004 (2004)

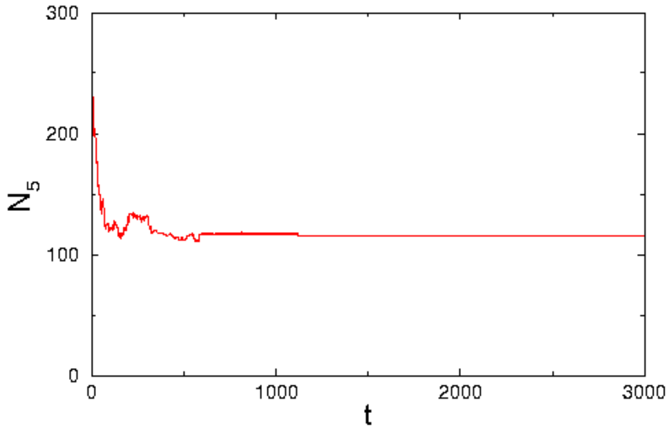
Weak pinning

I.V. Grigorieva, Sov. Phys. JETP **69**, 194 (89).

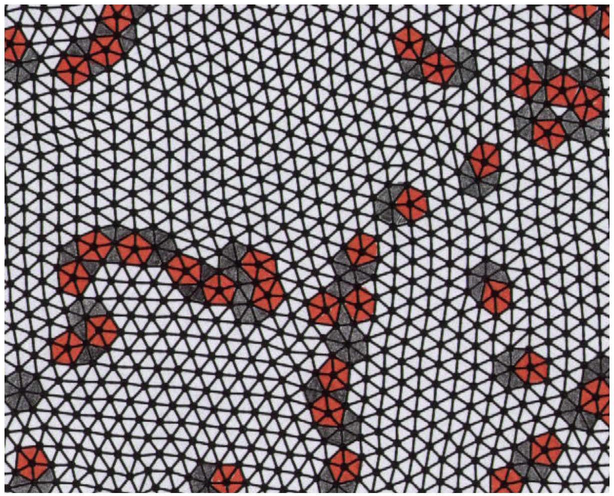
Vortex polycrystal

Numerical evidence

Vortex simulations of a rapid field cooling (FC) in the stripe geometry—weak or strong pinning.



- Initially, many dislocations annihilate and react with each other.
- Dislocations form GB's.
- Growth of grains with various sizes and orientations.
- Structure gets pinned by disorder.



Numerical analysis

N (up to 4128) vortices in a cell of size D (D 18,36,72λ).

Periodic boundary conditions.

Vortex mutual interactions:

$K_1(r_{ij}/\lambda)$ Bessel function → **$\sim r^{-1}$ if $r<\lambda$**; → **$\sim e^{-r}$ if $r<\lambda$**

λ London penetration length

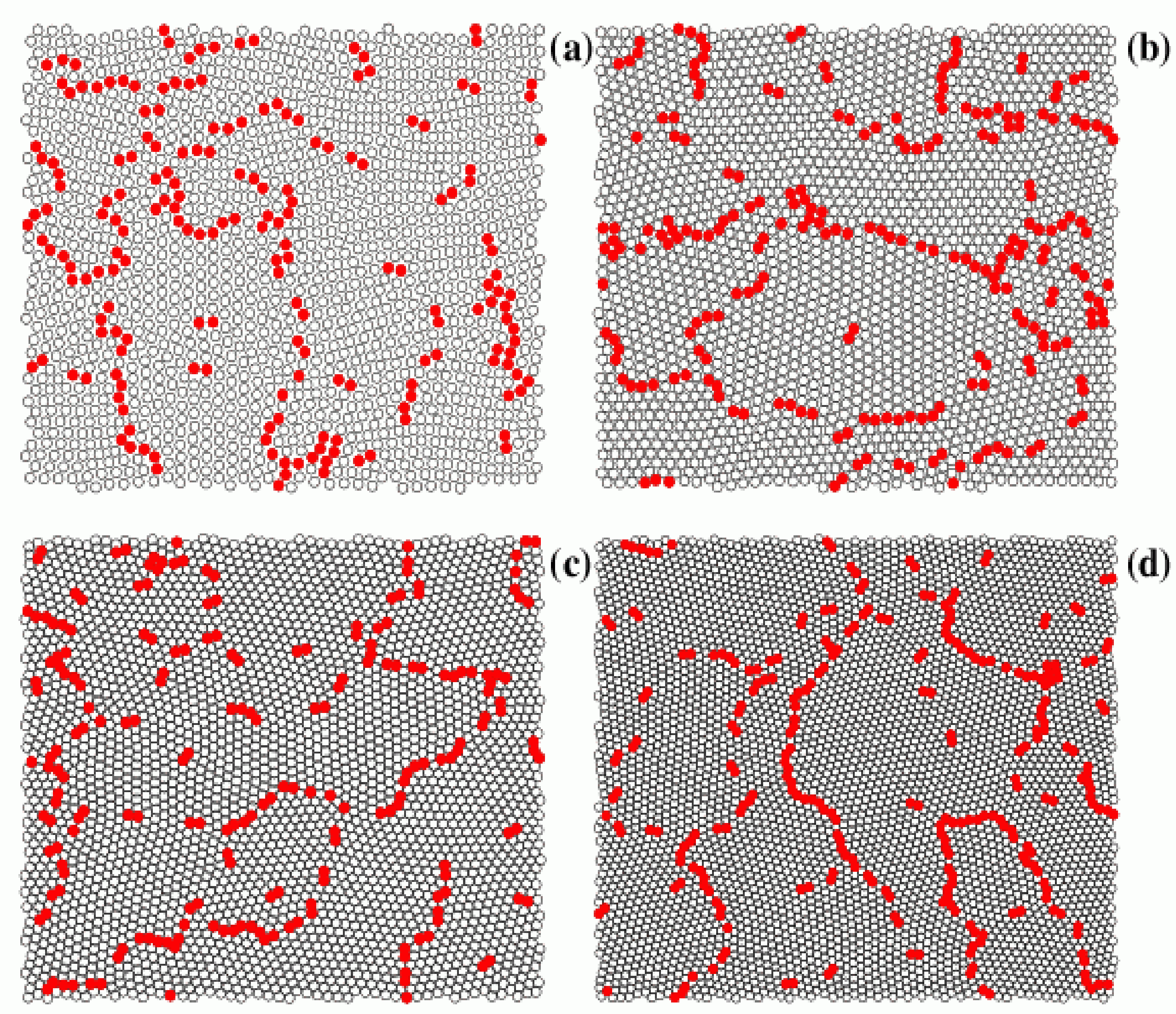
Point-like pinning centers.

Initial configuration: Random configuration of vortex lines.

- Keep track of vortex dynamics with or without current-ind. forces.
- Calculate lattice topology, current thresholds, etc.

Grain boundary pinning

Pinned vortex & dislocation structures.

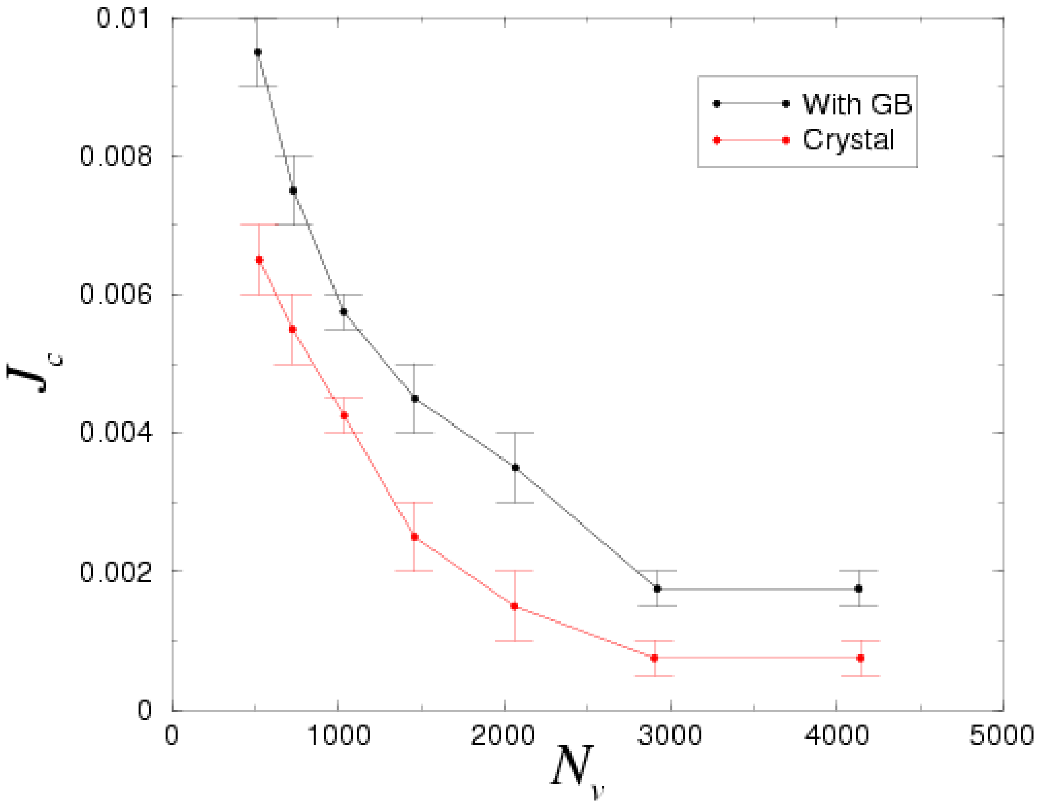


Increasing density of vortex lines from a) till d)

Depinning current with GB

- Grain boundaries also move in response to applied currents.

- Numerical data indicate:
  - If GB after field cooling: The depinning current J_c increases, i.e. it is above the single crystal value.
  - The critical current J_c may depend on the average grain size, as the yield stress for polycrystals (*Hall-Petch relation*).

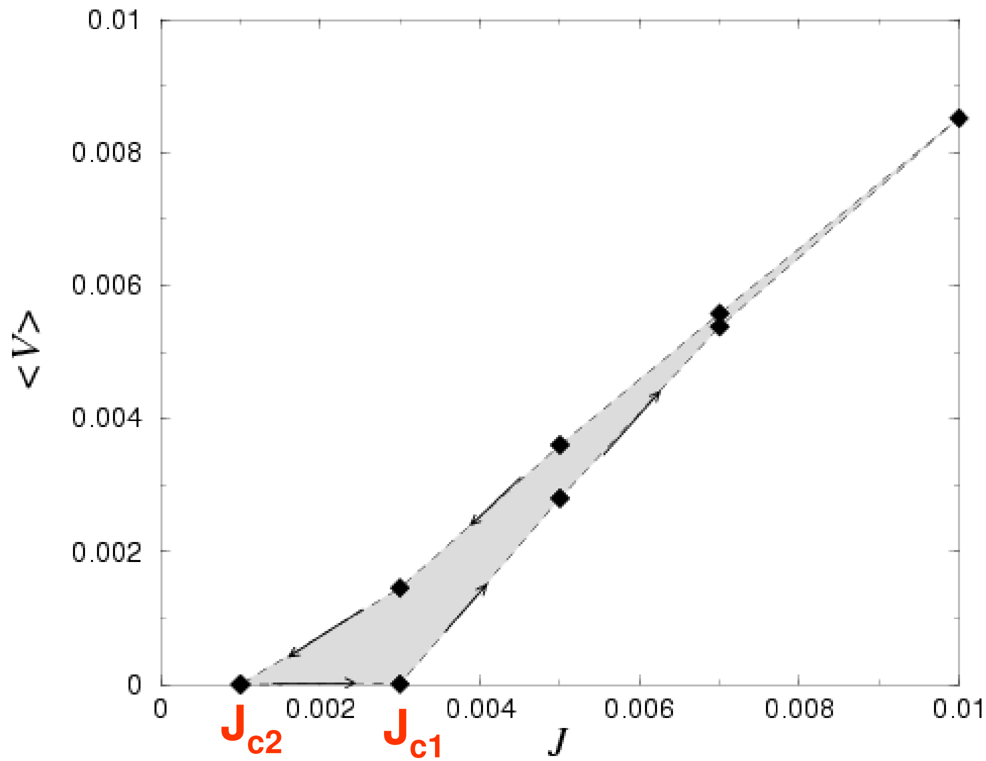


- Needs further study for different pinning regimes, cooling histories → average grain sizes, etc.

Hysteretic behavior

- Commonly observed in FC critical current measurements.

- Above depinning $J>J_c(B)$:
  - Plastic flow mediated by GB sliding.
- Metastability
  - Upon ramping up and down the driving current, the number of dislocations in GB decreases, and the critical current decreases from J_{c1} to J_{c2} .



In good agreement with transport experiments, i.e.

Z.L. Xiao et al., PRL **85**, 3265 (2000),

Z.L. Xiao et al., PRL **86**, 2431 (2001).

Conclusions

- Plastic avalanches in acoustic emission experiments and in 2D dislocation dynamic models (Andrade's creep, intermittency).
  - Power law distributions of plastic events.
  - Aftershock triggering & slowly decaying time correlations.

- Dislocation induced jamming transition in 2D dislocation dynamic models.
  - Analogous rheology in soft amorphous materials ⇒ *Jamming scenario*.

- Spatio-temporal heterogeneity of slip ⇒ Self-affine rough surfaces

- After standard field-cooling protocols, we observe vortex polycrystals where grain growth is limited by grain boundary pinning.
  - Elastic properties of grain boundaries: strongly non-local.
  - Estimates for the depinning stress and the average grain size, under weak and strong pinning assumptions.

- Increase of the critical depinning current for vortex polycrystals.
  - Hysteresis ⇒ Metastability.